SHORT COMMUNICATIONS

The Crystal Structure of *o*-Toluic Acid

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o-Toluic acid is an interesting substance, since a considerable steric hindrance between the methyl group and the carboxyl group in the same molecule can be anticipated. In order to obtain the three-dimensional configuration of this molecule, an X-ray investigation has been performed.

The crystal of this compound is monoclinic, with cell dimensions of $a=4.83$, $b=19.33$, $c=7.82$ Å, and $\beta=109.0°$. The space group is $P2_1/c$, and the unit cell contains four molecules. The calculated density is 1.30 g·cm^{-3}, and the observed value obtained by the floatation method is 1.29 g·cm^{-3}. As the three-dimensional data of intensities, 1230 reflections were measured visually from integrating Weissenberg photographs around the a and c axes taken with filtered Cu$K\alpha$ radiation.

The structure projections along the a and c axes were elucidated by means of the method of trial and error, and were refined by two-dimensional Fourier syntheses. The structure thus obtained was refined further by the three-dimensional least-squares method using isotropic temperature factors. The discrepancy index, R, is 16.8% at the present stage of refinement.

The electron density and the crystal structure elucidation projected along the a axis are shown in Figs. 1 and 2 respectively. From the atomic distances and the bond angles estimated with the present parameters, the following conclusions may be drawn. The displacements of the methyl and carboxyl groups from the benzene plane are not very large, and the molecule is almost planar as a whole. Further, the two molecules, linked in a dimer around a center of symmetry by two O–H···O hydrogen bonds with a distance of 2.63 Å, are approximately coplanar. The O(1)–C(7) and O(2)–C(7) bonds are 1.32 and 1.22 Å in length respectively; therefore, the former seems to be a single bond, and the latter, a double bond. The bond angles, O(2)-C(7)–C(1), C(7)–C(1)–C(2), and C(1)–C(2)–C(8), are distorted by about +4°, +2°, and +5° respectively from the normal angle of 120°, so the O(2)···C(8) distance is increased to 2.78 Å. This value is, however, considerably smaller than the sum of the van der Waals radii (3.4 Å).

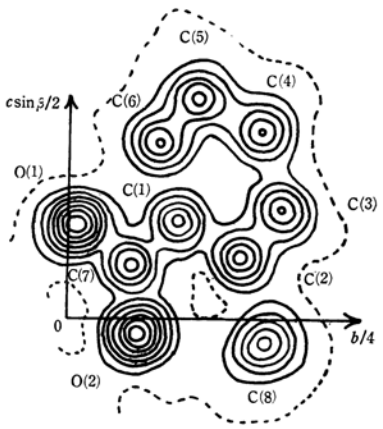

Fig. 1. Electron density along the a axis.

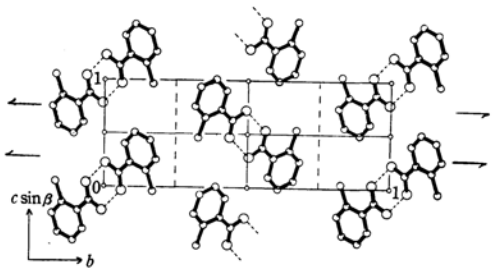

Fig. 2. Crystal structure along the a axis.