The Crystal Structure of *m*-Bromobenzoic Acid

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Ferguson *et al.*[1] have reported that the carboxyl group of ortho-substituted benzoic acid is twisted out of the benzene plane because of steric interaction between the carboxyl group and the substituent. The present investigation has been undertaken in order to elucidate the effect of the meta-substituent on the carboxyl group.

Crystal data were determined from Weissenberg and precession photographs as follows;

$a=25.99$ $b=4.73$ $c=6.07$ Å $\beta=102°$

space group $P2_1/a$

Equi-inclination Weissenberg photographs were taken for the layer lines from 0 to 3 about the b axis with Cu$K\alpha$ radiation. The structure was determined from Patterson maps and a three-dimensional electron density map. The positional and thermal parameters of each atom were refined by the least-squares method. After 3 cycles, the R factor was reduced to 0.11. The final parameters are tabulated in Table 1. The arrangement of molecules viewed along the b axis is shown in Fig. 1, which also includes the interatomic distances and angles.

The displacements of the atoms from the best plane of the molecule vary from 0.054 Å to −0.036 Å. These are not significant; thus, the carboxyl group is almost exactly coplanar with the benzene ring. The C–C distances in the benzene ring do not differ significantly from their mean value, 1.39 Å.

Two molecules, related to each other by a center of symmetry, form a dimer by means of the hydrogen bonds, OH···O, of 2.60 Å. Other intermolecular approaches are normal van der Waals contacts; the shortest are 3.44 Å between a carbon and oxygen atom, and 3.48 Å between carbon atoms.

Table 1. Atomic parameters

Atom	x/a	y/b	z/c	B(Å^{-2})
Br	0.2198	0.1003	0.7588	4.20
O(1)	0.0559	0.8294	0.6377	4.30
O(2)	0.0107	0.7849	0.2890	4.73
C(1)	0.0495	0.7246	0.4443	3.99
C(2)	0.0873	0.5088	0.3947	3.70
C(3)	0.1285	0.4289	0.5723	3.19
C(4)	0.1638	0.2279	0.5255	5.17
C(5)	0.1585	0.1093	0.3110	4.04
C(6)	0.1171	0.1743	0.1468	3.79
C(7)	0.0817	0.3899	0.1886	3.67

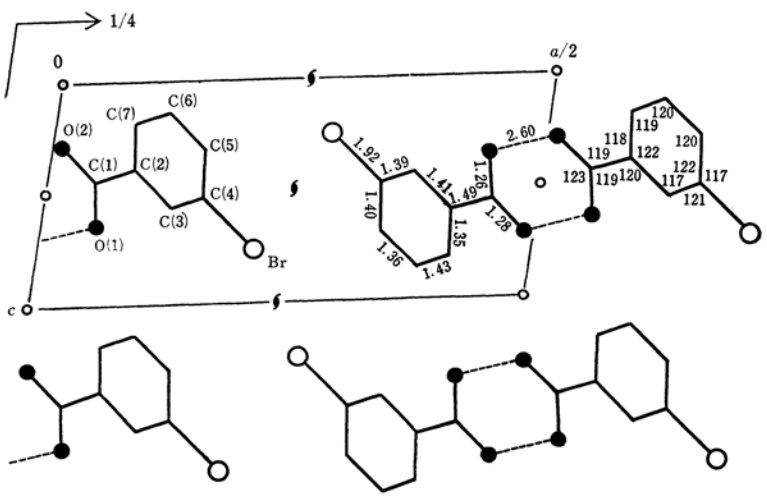

Fig. 1. The crystal structure viewed along the b axis. Bond distances (Å) and angles (°) are shown. The broken line shows the hydrogen bond.

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1) G. Ferguson and G. A. Sim, *Acta Cryst.*, **14**, 1262 (1961).