Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1963). **16**, 313

The structure of *m*-bromonitrobenzene.

By T. L. CHARLTON and J. TROTTER, *Department of Chemistry, University of British Columbia, Vancouver 8, Canada*

(*Received* 18 *May* 1962 *and in revised form* 14 *September* 1962)

Crystals of *m*-bromonitrobenzene are colourless prisms elongated along *c*, and are quite volatile. Crystal data were determined as usual, using samples sealed in Lindemann glass capillaries (Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å):

$C_6H_4NO_2Br$; $M = 202{\cdot}0$; m.p. = 56 °C.
Orthorhombic, $a = 5{\cdot}92$, $b = 21{\cdot}52$, $c = 5{\cdot}34$ Å.
Volume of the unit cell = 680·3 Å^3.
D_c (with $Z = 4$) = 1·960, $D_{meas} = 1{\cdot}93$ g.cm.$^{-3}$ (flotation in aqueous $AgNO_3$).
Absorption coefficients for X-rays:
$\mu = 81$ cm.$^{-1}$ (Cu), $\mu = 65$ cm.$^{-1}$ (Mo).
$F(000) = 392$.
Absent spectra: $0kl$ when k is odd, $h0l$ when $(h+l)$ is odd.
Space group is $Pbn2_1$ or $Pbnm$; $Pbn2_1$ was confirmed by the structure analysis.

The structure was determined from Patterson, electron-density and difference projections along the *a*- and *c*-axes, with 63 $0kl$ reflexions ($R = 0{\cdot}14$) and 114 $hk0$ reflexions ($R = 0{\cdot}14$) (structure factor data are available from the authors). The final positional (fractions of cell edges) and thermal parameters are listed in Table 1, together with the displacements of the atoms from a plane through the six carbons. These latter indicate that the molecule is planar within experimental error.

Table 1. *Final positional and thermal parameters, and deviations* (Δ) *from the mean plane*

Atom	*x*	*y*	*z*	*B* (Å^2)	Δ (Å)
Br	0·0412	0·2370	0·0000	4·5	−0·04
C_1	0·1872	0·1707	0·1625	4·5	−0·02
C_2	0·0760	0·1440	0·3659	4·5	+0·02
C_3	0·1812	0·0937	0·4766	4·5	−0·02
C_4	0·3972	0·0720	0·4137	4·5	+0·02
C_5	0·5034	0·1004	0·2081	4·5	−0·02
C_6	0·3988	0·1499	0·0985	4·5	+0·02
N	0·0650	0·0651	0·6875	4·5	+0·01
O_1	−0·1207	0·0828	0·7607	5·0	+0·02
O_2	0·1462	0·0230	0·8086	5·0	+0·05

Differences between chemically similar bonds and angles are not significant, the mean values of the bond lengths being, with e.s.d.'s (Cruickshank, 1949): Br–C = 1·88 ± 0·05, C–C = 1·39 ± 0·03, C–N = 1·46 ± 0·07, N–O = 1·22 ± 0·04 Å.

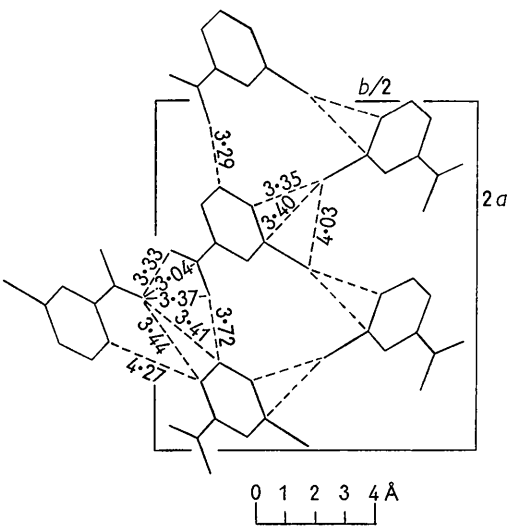

Fig. 1. Projection of the structure onto (001), showing the shorter intermolecular distances.

There are two unusually short intermolecular Br–C contacts (3·35 and 3·40 Å), the Br atom of each molecule being situated almost exactly above the centre of, and at a distance of 3·30 Å from, the C_1–C_6 bond of a second molecule, suggesting charge-transfer bonding (Charlton & Trotter, 1962). All the other contacts (Fig. 1) correspond to normal van der Waals interactions.

The authors thank the National Research Council of Canada and the President's Research Fund, University of British Columbia, for financial support, Dr F. R. Ahmed for kindly making available his IBM 1620 programs, and the staff of the University of British Columbia Computing Centre for assistance with the operation of the computer.

References

CHARLTON, T. L. & TROTTER, J. (1962). *Proc. Chem. Soc.*, p. 221.
CRUICKSHANK, D. W. J. (1949). *Acta Cryst.* **2**, 65.