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The crystal structure of 2-amino-5-bromotoluene.

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2-Amino-5-bromotoluene crystallizes in space group $P2_12_12_1$ with cell constants $a=15.265$, $b=8.756$, $c=5.578$ Å and four molecules in the unit cell.

Dr H. F. van Woerden from the Laboratory for Organic Chemistry of the University of Amsterdam prepared various substituted thionylanilines (Michaelis & Herz, 1890; van Woerden,personal communication) by reaction of the parent aniline derivative with $SOCl_2$. One of these, 2-methyl-4-bromothionylaniline, was selected for a crystal structure determination. However, from the result of the structure determination and the fact that thionylanilines easily undergo hydrolysis to the corresponding anilines (van Woerden, personal communication), it was concluded that on recrystallization in order to get suitable crystals for the intensity measurements the hydrolysis product 2-amino-5-bromotoluene had been obtained. Because the crystal structure of this simple compound could not be found in the literature (Kennard & Watson, 1971), it is briefly reported here.

The cell constants, determined from Weissenberg photographs calibrated with Al-powder lines, are $a=15{\cdot}265$ (3), $b=8{\cdot}756$ (3), $c=5{\cdot}578$ (1) Å; the space group is $P2_12_12_1$; with $Z=4$ the calculated density is 1·66 g. cm^{-3}. With an automatic Nonius single-crystal diffractometer, 542 non-zero intensities were observed up to $\theta=55°$ with Ni-filtered Cu K radiation and operating in the θ–2θ scan mode.

The position of the bromine atom was readily determined from the Patterson function. A minimum function based on the bromine position, although complicated by a pseudo mirror plane perpendicular to the c axis owing to the small distance of the bromine atom from $z=\frac{1}{4}, \frac{3}{4}$, revealed the positions of all the carbon and nitrogen atoms.

The structure was refined to $R=0{\cdot}081$ with anisotropic temperature parameters for the bromine and isotropic ones for the light atoms. No further refinement was carried out. In Table 1, the coordinates and temperature parameters are given; Fig. 1 shows the bond lengths and bond angles (standard deviations estimated as 0·03 Å and 2° respectively) and Fig. 2 the structure projected along [001].

Table 1. *Fractional coordinates* ($\times 10^4$) *and temperature parameters* (Å^2)

$\beta_{ij}=2\pi^2 a_i^* a_j^* U_{ij} \times 10^4$.

Estimated standard deviations are in parentheses.

	x	y	z	B_{iso}
Br(1)	9870 (01)	−0367 (03)	7282 (06)	
C(2)	9052 (13)	0964 (20)	5975 (40)	4·5 (4)
C(3)	8220 (13)	1148 (20)	7130 (38)	4·6 (4)
C(4)	7592 (11)	2110 (17)	6236 (34)	3·8 (3)
C(5)	7791 (11)	2938 (18)	4116 (34)	3·4 (3)
C(6)	8631 (13)	2782 (20)	2913 (40)	4·8 (4)
C(7)	9199 (12)	1755 (20)	3953 (38)	4·7 (4)
C(8)	6723 (15)	2270 (22)	7308 (42)	5·1 (4)
N(9)	7187 (13)	4031 (19)	3268 (38)	5·9 (4)

β_{11}	β_{22}	β_{33}	$2\beta_{12}$	$2\beta_{23}$	$2\beta_{13}$
55 (1)	264 (5)	644 (12)	46 (3)	64 (12)	−15 (6)

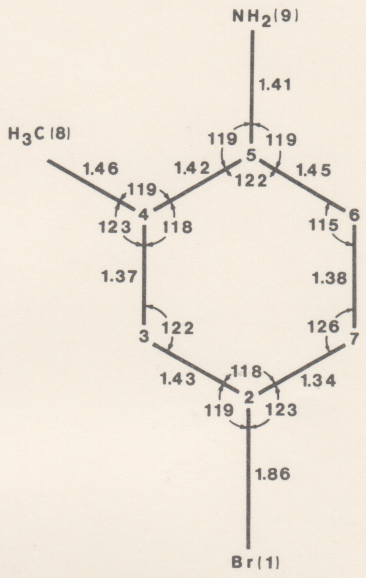

Fig. 1. Numbering of atoms, bond lengths and bond angles.

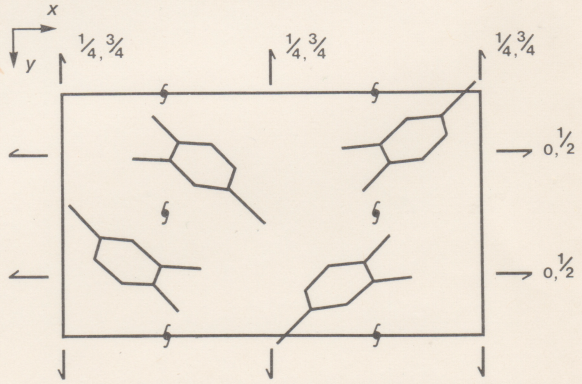

Fig. 2. Projection of the structure along [001].

The distance between the bromine and the nitrogen atom of the two molecules related by a twofold screw axis in the [100] direction is 3·74 Å.

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