pycnometric density has not been determined. Since the sizes of the chlorine and bromine atoms do not differ very much, it may be concluded from an examination of the lattice constants that there are four molecules in the H_3CCN–BBr_3 unit cell, giving for the X-ray density 2·65 g.cm.$^{-3}$.

It is strongly indicated that these methyl cyanide–boron trihalides are isomorphous (space group *Pnma*). However, we have decided not to continue the investigations of the structures of the chlorine and bromine compounds since we feel that the heavy atoms bonded to the boron atom would not permit a highly accurate determination of the boron position.

This work was supported by the Office of Naval Research, Contract No. N6ori-91, Task Order 4, Project No. NR 052020.

References

HOARD, J. L., OWEN, T. B., BUZZELL, A. & SALMON, O. N. (1950). *Acta Cryst.* **3**, 130.

LAUBENGAYER, A. W. & SEARS, D. S. (1945). *J. Amer. Chem. Soc.* **67**, 164.

Acta Cryst. (1951). **4**, 380

Note on the crystalline structure of trimethylamine–borine, $(H_3C)_3N$–BH_3.

By S. GELLER,* R. E. HUGHES and J. L. HOARD, *Baker Laboratory of Chemistry, Cornell University, Ithaca, N.Y., U.S.A.*

(*Received* 26 *January* 1951)

Prof. G. W. Schaeffer, of St Louis University, kindly supplied us with the trimethylamine–borine used in our structural study. The vapor pressure of $(H_3C)_3N$–BH_3 is high enough to permit growing of crystals in thin-walled glass capillaries by the technique employed for H_3CCN–BF_3 (Hoard, Owen, Buzzell & Salmon, 1950) and $(H_3C)_3N$–BF_3 (Geller & Hoard, 1951), but we have been unable to grow specimens sufficiently large and well crystallized to provide adequate diffraction data for an accurate determination of structure. Data of rather poor quality, obtained with Cu $K\alpha$ radiation from one crystal, have led to the following results.

The symmetry of the X-ray patterns corresponds to D_{3d}–$\bar{3}m$. The hexagonal unit of structure has

$$a = 9{\cdot}33 \pm 0{\cdot}05, \quad c = 5{\cdot}90 \pm 0{\cdot}05\,\text{A.},$$

and contains three molecules (X-ray density, 0·82 g.cm.$^{-3}$). However, the data are also consistent with a one-molecule rhombohedral unit having

$$a = 5{\cdot}74\,\text{A.}, \quad \alpha = 109°.$$

With no special vanishings and lattice constants very similar to those of trimethylamine–boron trifluoride, isomorphism of $(H_3C)_3N$–BH_3 and $(H_3C)_3N$–BF_3 is strongly indicated. This conclusion is supported further by a comparison between observed and calculated amplitudes for (*HK*.0) reflections. Nitrogen and boron atoms lie on the threefold axis and carbon atoms lie in the vertical symmetry planes of C_{3v}^5–$R3m$. The x parameter of the carbon atom is approximately the same as in the $(H_3C)_3N$–BF_3 structure, namely, −0·090. The comparison between calculated and observed amplitudes (B taken equal to 2·5 A.^{2} as in $(H_3C)_3N$–BF_3) for (*HK*.0) reflections is shown in Table 1.

Table 1. *Calculated and observed reflection amplitudes*

(*HK*.0)	$\lvert F_c \rvert$	$\lvert F_o \rvert$
03.0	22	18
06.0	5	11
09.0	4	<2
11.0	39	34
14.0	13	21
17.0	7	7
22.0	8	8
25.0	13	15
28.0	2	<2
33.0	19	20
36.0	8	8
44.0	17	16
47.0	4	1
55.0	5	6
66.0	2	<1

It is possible that other methods of obtaining crystals and the use of low-temperature equipment (not at present available in this Laboratory) would yield X-ray data of better quality.

An electron-diffraction investigation of the structure of $(H_3C)_3N$–BH_3 was made by Bauer (1937), in which the B–N distance was found to be 1·62 ± 0·15 A. The following considerations imply that the value obtained by Bauer is correct within much narrower limits than he indicated. The B–N distance covering the range of most probable values in the compounds H_3CH_2N–BF_3 (Geller & Hoard, 1950), $(H_3C)_3N$–BF_3, H_3N–BF_3 (Hoard, Geller & Cashin, 1951) is 1·585 ± 0·015 A. These compounds are comparable in stability with $(H_3C)_3N$–BH_3.

References

BAUER, S. H. (1937). *J. Amer. Chem. Soc.* **59**, 1804.

GELLER, S. & HOARD, J. L. (1950). *Acta Cryst.* **3**, 121.

GELLER, S. & HOARD, J. L. (1951). *Acta Cryst*, **4**, 399.

HOARD, J. L., GELLER, S. & CASHIN, W. M. (1951). *Acta Cryst.* **4**, 396.

HOARD, J. L., OWEN, T. B., BUZZELL, A. & SALMON, O. N. (1950). *Acta Cryst.* **3**, 130.

* duPont Post-Doctoral Fellow, 1949–50. Present address: E. I. duPont de Nemours and Co., Rayon Department, Acetate Research, Waynesboro, Virginia, U.S.A.