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The structure of hydrazinium fluoborate.

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Hydrazinium fluoborate, NH_2–$NH_3^+BF_4^-$ crystallizes in a monoclinic form in space group $C2/c$ (or Cc). The unit-cell dimensions and atomic positional parameters x and z are reported here.

Hydrazinium fluoborate was prepared by neutralizing a 15% solution of hydrazine in 2-propanol with a 50% aqueous solution of fluoboric acid to a methyl red end-point. The product solution was evaporated to dryness and the residue recrystallized from 2-propanol. The crystals appeared as blunt rods elongated parallel to the unique axis, b.

Rotation and Weissenberg photographs around b were taken with Cu $K\alpha$ radiation. The length of the b axis was estimated from the rotation diagram and the parameters a, c and β were taken from the Weissenberg films. The resulting values (based on λ Cu $K\alpha = 1{\cdot}5418$ Å) and their estimated standard deviations are:

$$a = 14{\cdot}17 \pm 0{\cdot}02,\ b = 5{\cdot}25 \pm 0{\cdot}10,\ c = 12{\cdot}58 \pm 0{\cdot}03 \text{ Å};$$
$$\beta = 113{\cdot}1 \pm 0{\cdot}5°.$$
$$\text{Cell volume} = 855{\cdot}6 \text{ Å}^3.$$
$$D_x = 1{\cdot}86 \text{ g.cm}^{-3} \text{ for } Z = 8.$$

The systematic absences of hkl with $(h+k)$ odd, and $h0l$ with l odd suggest that the structure belongs in space group $C2/c$ (No. 15) or Cc (No. 9). We have assumed the former.

A crystal with cross section 0·4 × 0·4 mm was cleaved to a length of 0·6 mm and was mounted in a glass capillary with the rotation axis parallel. This crystal was used for the preparation of three-film Weissenberg photographs of the $h0l$ layer. The intensities were estimated visually by comparison with a calibrated strip prepared from the same crystal, and were adjusted for the Lorentz and polarization effects. A sharpened vector map with the origin suppressed was made with the Patterson function. The x and z trial parameters of the (010) projection were determined from the vector map and from knowledge of the probable molecular configuration.

They were refined by use of the Gantzel, Sparks & Trueblood (1961) Least Squares Refinement Program for the IBM 7090 computer. An isotropic temperature factor was refined for each atom. The hydrogen atoms were not considered. After five least-squares cycles, R minimized at 21%. The resulting parameters are shown in Table 1.

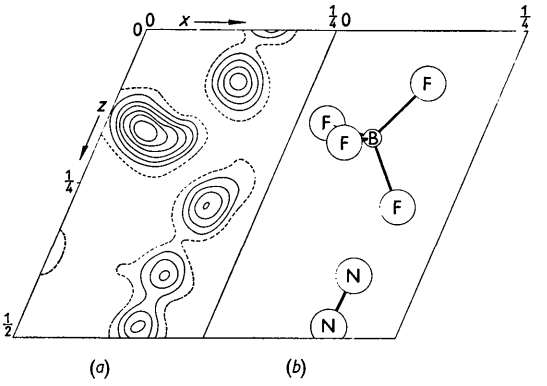

Fig. 1. (*a*) Electron density projection onto (010). The contours are at intervals of 1 e.Å^{-2}. (*b*) Possible orientation of hydrazinium and fluoborate ions.

Table 1. *Atomic parameters*

Atom	x	z	Isotropic temperature factor
B	0·104	0·174	0·53 Å^2
F(1)	0·178	0·284	3·04
F(2)	0·072	0·181	3·42
F(3)	0·039	0·150	2·59
F(4)	0·149	0·085	2·57
N(1)	0·156	0·479	1·47
N(2)	0·159	0·396	2·73

No further work is scheduled for this structure.

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Reference

GANTZEL, P. K., SPARKS, R. A. & TRUEBLOOD, K. N. ACA Computer Program No. 317 (UCLASF 1).

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