

complexed the ether released; this shifted the equilibrium and permitted the isolation of formerly unattainable  $F_2XP \cdot B_3H_7$  and  $OCB_3H_7$  complexes. Stability data suggest that if a relatively strong base is bound to the  $B_3H_7$  fragment, the *acid strength* of the base- $B_3H_7$  complex is inductively reduced.<sup>4,6,13</sup> Under these conditions, attack can only be by a very strong Lewis base. For this reason the  $(CH_3)_3N \cdot B_3H_7$  complex, when once formed, is attacked only by excess  $(CH_3)_3N$  or, better, by still stronger bases [*i.e.*,  $P(C_6H_5)_3$ ].

As noted above, the equilibrium in the reversible displacement reaction (eq 1 and 2) is important. If the attacking base (L) is much stronger than the base which is being displaced (*i.e.*,  $(CH_3)_2O$ ), the equilibrium in the 1:1 mixture goes rapidly to completion and the concentration of free base (L) capable of attacking the  $LB_3H_7$  complex is reduced effectively to zero, thus minimizing conversion to  $L_2 \cdot B_2H_4$  through eq 3. This is observed when L is  $(CH_3)_3N$ .<sup>13</sup> Since the  $(CH_3)_3N \cdot B_3H_7$  complex is stable enough to resist attack by ether, further decomposition does not occur.

In the case of the reaction of  $PF_2X$  and  $(CH_3)_2O \cdot B_3H_7$ , conversion to  $(F_2XP)_2 \cdot B_2H_4$  is promoted by the moderately high residual acid strength of the complex  $F_2XP \cdot B_3H_7$  and by the high equilibrium concentration of  $F_2XP$  in the initial displacement process. The foregoing model suggests that as the attacking base  $F_2XP$  becomes weaker, the concentration of  $F_2XP \cdot B_3H_7$  should decrease. This is in complete agreement with published work; *e.g.*, the decreasing base strength trend  $X = (CH_3)_2N > F > Cl > Br$  parallels the decreasing stability of  $F_2XP \cdot B_3H_7$ .<sup>6</sup> Furthermore the presence of uncoordinated fluorophosphine in increasing equilibrium amounts in the order  $X = (CH_3)_2N > F > Cl, Br$  should result in increasing degradation of the  $F_2XP \cdot B_3H_7$  and increasing amounts of  $(F_2XP)_2 \cdot B_2H_4$ . Analysis of the product yields from the 1:1 reaction of  $(CH_3)_2O \cdot B_3H_7$  and  $F_2XP$ , in fact, shows a small relative increase in the amount of  $(F_2XP)_2 \cdot B_2H_4$  formed with decreasing base strength. Clearly, as noted by Ritter and his associates, both the relative strength of the bases which determine concentrations in the displacement reactions and the absolute strength of bases which determine strength of the base- $B_3H_7$  complex as a Lewis acid are important in determining products to be expected from these reactions.

The reactions of  $B_4H_{10}$  can be treated in a strictly analogous manner if a  $BH_3$  group, coordinating through a double BHB bridge, is considered as an operational Lewis base comparable to  $(CH_3)_2O$ .<sup>5</sup> Indeed, these reactions of  $B_4H_{10}$  with a 2 mol sample of base can be considered as one of the first cases of an assisted displacement reaction since the operational base,  $BH_3$ , is tied up by the Lewis base  $NR_3$  and removed from the system just as effectively as  $(CH_3)_2O$  is removed by  $BF_3$ .<sup>6</sup>

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**Registry No.**  $(F_3P)_2 \cdot B_2H_4$ , 17239-60-0;  $(F_2ClP)_2 \cdot B_2H_4$ , 53293-17-7;  $(F_2BrP)_2 \cdot B_2H_4$ , 53229-22-4;  $B_4H_{10}$ , 18283-93-7;  $(CH_3)_2O \cdot B_3H_7$ , 53229-23-5;  $PF_3$ , 7783-55-3;  $PF_2Cl$ , 14335-40-1;  $PF_2Br$ , 15597-40-7.

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## Photochemical Reaction of Hexafluoroacetone with Borazine. Preparation of *B*-(2*H*-Hexafluoro-2-propoxy)borazine and *B*-(Perfluoro-*tert*-butoxy)borazine

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Photochemical reactions of borazine in the absence of photosensitizing reagents have been interpreted as proceeding through an excited-state mechanism when borazine is the primary absorber.<sup>1-3</sup> Reactions involving free-radical intermediates have not been explored as potential sources of new borazine derivatives. We have now investigated the reaction of borazine in the presence of photochemically generated radicals from hexafluoroacetone (HFA). The photochemistry of HFA has been the subject of numerous studies,<sup>4-6</sup> and quantitative data for fluorescence<sup>5b,7</sup> and phosphorescence<sup>5b,6</sup> rate constants have been reported. Electronic excitation of borazine is observed at wavelengths below 2000 Å.<sup>8-11</sup> Thus, in mixtures of borazine and HFA, photolysis at wavelengths above 2000 Å will be controlled primarily by HFA intermediates. Two reports in the literature describe the photolysis of HFA with diborane<sup>12</sup> and with triethylborane.<sup>13</sup> However, the boron-containing products of these reactions were not identified.

## Experimental Section

Borazine was prepared by the reduction of *B*-trichloroborazine with  $NaBH_4$  (Alpha Chemical Co.) according to the method of Hohnstedt and Haworth.<sup>14</sup> *B*-Trideuterioborazine was prepared by the photolysis of borazine with excess  $D_2$  (Matheson, CP grade, 99.5 atom %).<sup>1</sup> Hexafluoroacetone (Matheson), 2*H*-hexafluoro-2-propanol (E. I. du Pont de Nemours and Co., Inc.), and perfluoro-*tert*-butyl alcohol (Peninsula ChemResearch) were vacuum distilled through a trap maintained at  $-80^\circ$ . Purity of these reagents was confirmed by infrared and mass spectra.

Photolyses of borazine-HFA mixtures (4:1 molar ratio, total pressure 5 mm) were carried out in a 2-l. vessel equipped with a quartz immersion well. The light source, a Hanovia medium-pressure mercury lamp, was purged with dry nitrogen during the 25-min photolysis periods. In separate experiments Vycor and Correx filters were used to block radiation below 2200 and 2700 Å, respectively. In one experiment, *B*-trideuterioborazine was photolyzed with HFA. The photochemical products were separated by conventional vacuum distillation through traps maintained at  $-55$ ,  $-65$ , and  $-196^\circ$ . The  $-55^\circ$  trap was found to contain a new photochemical product subsequently identified as I, while analysis of the  $-65^\circ$  trap revealed a mixture of I and a slightly more volatile product II. These products were obtained under all light filter conditions employed. Products I and II were also obtained in pure form by 1849-Å photolysis of hexafluoro-2-propanol-borazine and perfluoro-*tert*-butyl alcohol-borazine mixtures, respectively. For the latter experiments borazine-alcohol mixtures in a 4:1 ratio (total pressure 5 mm) were photolyzed for 30 min. In order to clarify the reaction mechanism, product I was photolyzed for 30 min with HFA. Neither I nor II is observed as a thermal product at the pressures studied. Products were analyzed by mass, infrared, and nmr spectroscopy. Mass spectra

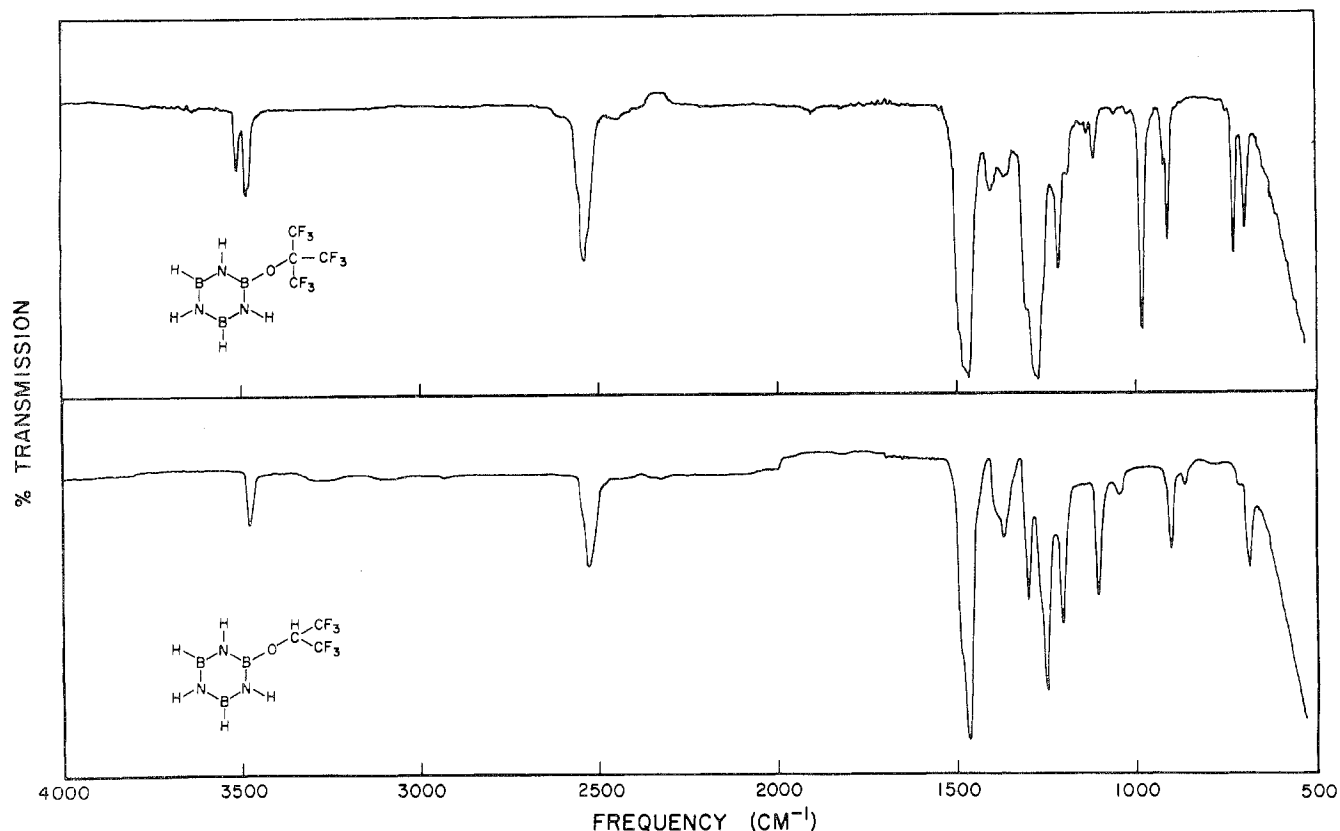


Figure 1. Infrared spectra of photochemical products *B*-(perfluoro-*tert*-butoxy)borazine (top) and *B*-(2*H*-hexafluoro-2-propoxy)borazine (bottom).

were obtained on a Perkin-Elmer MS 270. Infrared spectra of gas samples at about 2 mm (vapor pressure at 20°) were obtained on a Perkin-Elmer 521 infrared spectrophotometer. Proton nmr samples (10% solutions in CDCl<sub>3</sub>) were analyzed on a Bruker HX-90 with FTS/NMR Pulser 400-2 (90 MHz) connected to a Digilab Nova computer. With a deuterium lock (CDCl<sub>3</sub>) the 250-Hz region was scanned 1200 times, using a pulse width of 5.0 μsec and a 4-sec delay time. The 0.2% CHCl<sub>3</sub> impurity in the CDCl<sub>3</sub> was used as a reference peak. A Varian HA-100 nmr was used for both the <sup>11</sup>B and <sup>19</sup>F nmr spectra, with external reference compounds trimethyl borate and trifluoroacetic acid, respectively. All proton chemical shifts reported here have been converted to δ<sub>TMS</sub> values by the formula δ<sub>TMS</sub> = 7.28 - δ<sub>CHCl<sub>3</sub></sub>; the <sup>19</sup>F chemical shifts are given as δ<sub>CFCl<sub>3</sub></sub>, where δ<sub>CFCl<sub>3</sub></sub> = δ<sub>CF<sub>3</sub>COOH</sub> - 78.50; and the <sup>11</sup>B chemical shifts are referenced to B(OCH<sub>3</sub>)<sub>3</sub>. In all cases the downfield shifts are taken as positive. The contents of the -196° trap were identified by their infrared spectra.

**Product I, H<sub>2</sub>((CF<sub>3</sub>)<sub>2</sub>HCO)B<sub>3</sub>N<sub>3</sub>H<sub>3</sub>.** The mass spectrum of this compound indicated the following ion intensities in the high-mass region: *m/e* (intensity) 248 (6), 247 (87), 246 (100), 245 (42), 244 (11), 178 (59), 177 (48), 176 (18). This pattern is consistent with a parent mass of 247 for the <sup>11</sup>B<sub>3</sub> species. A mass grouping between 178 and 176 is interpreted as loss of a CF<sub>3</sub> group on fragmentation. The parent mass of the product obtained from photolyses of *B*-trideuterioborazine-HFA mixtures was shifted upward 3 mass units to *m/e* 250. The infrared spectrum of I (Figure 1) is typical of *B*-monosubstituted borazines. Frequencies of the major bands in cm<sup>-1</sup> are as follows: 3481 (m), 2939 (w), 2533 (m), 1470 (s), 1374 (w), 1305 (m), 1254 (s), 1210 (m), 1113 (m), 910 (m), 692 (m). A weak C-H stretching frequency is observed at 2939 cm<sup>-1</sup>. This band is absent in the product obtained from *B*-trideuterioborazine. The strong band at 1254 cm<sup>-1</sup> is probably the B-O stretching vibration. The characteristic absorptions due to CF<sub>3</sub> groups are observed in the frequency range 1350-1100 cm<sup>-1</sup>. The proton nmr spectrum of I shows a septet at 4.56 ppm downfield from TMS and a coupling constant *J*<sub>HF</sub> = 5.75 ± 0.01 Hz. The <sup>19</sup>F nmr spectrum consists of a doublet at -75.23 ppm with *J*<sub>HF</sub> = 5.75 ± 0.12 Hz. The <sup>11</sup>B nmr spectrum indicates a singlet at 8.7 ppm and a doublet (*J* = 130 Hz) at 15.6 ppm downfield from trimethyl borate.

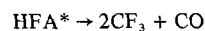
**Product II, H<sub>2</sub>((CF<sub>3</sub>)<sub>3</sub>CO)B<sub>3</sub>N<sub>3</sub>H<sub>3</sub>.** A mass spectrum of product II in the high, parent mass region showed the following ion intensity pattern: *m/e* (intensity) 316 (1), 315 (11), 314 (51), 313 (62), 312 (29). Mass groupings between 246 and 244 and between 276 and 273 indicate fragmentation by loss of CF<sub>3</sub> and by combinations of F and HF, respectively. The mass spectrum of the product obtained by photolysis with *B*-trideuterioborazine indicated the parent mass had increased by 2 units. The major infrared absorption bands for II occur at the frequencies 3511 (m), 3485 (m), 2540 (m), 1467 (s), 1272 (s), 1214 (m), 1118 (w), 983 (s), 912 (m), 730 (m), and 700 (m) cm<sup>-1</sup>. The spectrum (Figure 1) shows an obvious splitting of the N-H ring frequencies (3511 and 3485 cm<sup>-1</sup>) that is not typical of spectra of most *B*-monosubstituted borazine derivatives reported. The <sup>19</sup>F spectrum shows a singlet at -72.45 ppm. The <sup>11</sup>B nmr reveals a singlet at 8.7 ppm and a doublet (*J* = 130 Hz) at 15.6 ppm downfield from trimethyl borate.

A third component of the reaction products of HFA-borazine photolyses was collected in the -55° trap. The proportion of this product relative to I increased when the ratio of HFA to borazine in the photolysis mixture increased. Although II was not formed when I was photolyzed with HFA, this third component was a major product of that reaction. The <sup>19</sup>F nmr spectrum of this compound showed a doublet (δ -75.76 ppm) close to that observed for I and the <sup>1</sup>H nmr spectrum showed a septet (δ 4.90 ppm). This information and a resonance in the <sup>11</sup>B nmr spectrum at δ 2.9 ppm enabled us to identify this product as the borate B(OCH(CF<sub>3</sub>)<sub>2</sub>)<sub>3</sub> which probably results from thermal decomposition of photochemically generated borazine derivatives with two or three hexafluoropropoxy substituents. This behavior would be expected when the proportion of HFA in the reaction mixture is high and further ring substitution of I is likely. This is also consistent with the formation of the borate when I was photolyzed with HFA. The identity of this compound was confirmed by infrared and <sup>11</sup>B nmr spectra of B(OCH(CF<sub>3</sub>)<sub>2</sub>)<sub>3</sub> prepared by the reaction of diborane(6) with 2*H*-hexafluoro-2-propanol.

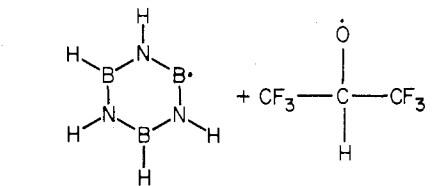
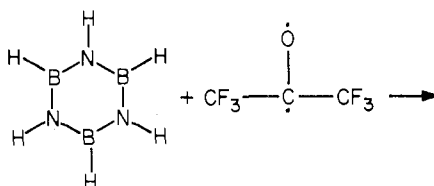
The content of the -196° trap was analyzed by infrared spectroscopy and found to contain C<sub>2</sub>F<sub>6</sub> and unreacted borazine. An infrared spectrum of the borazine recovered from experiments with *B*-trideuterioborazine indicated some H-D exchange had occurred on the borazine ring.

## Discussion

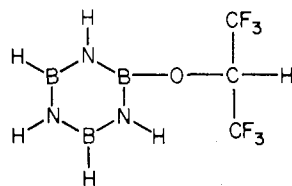
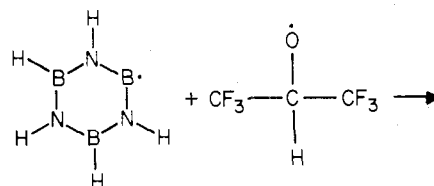
Photolysis of HFA-borazine mixtures with radiation above  $\lambda$  2200 Å yields two borazine derivatives shown by infrared, mass, and nmr spectra to be *B*-(2*H*-hexafluoro-2-propoxy)borazine and *B*-(perfluoro-*tert*-butoxy)borazine. Verification of the identity of these structures was obtained by preparing them separately by a photochemical reaction of borazine with the appropriate alcohol precursor under conditions where the mechanism involves excitation of the borazine molecule.<sup>15</sup> The photochemical mechanism for the HFA-borazine reactions with filtered light at wavelengths above 2200 or 2700 Å must involve excited HFA intermediates (HFA\*). The rates of the reactions of HFA\* with borazine are competitive with the photochemical decomposition process



which is the source of the relatively small quantities of  $\text{C}_2\text{F}_6$  produced. Quantitative photochemical studies have shown that the rate constant for the radiative decay of the singlet state of HFA is about 2 orders of magnitude slower than the rate constant for the nonradiative decay to the triplet state.<sup>16</sup> Under the low-pressure conditions of our experiments, the molecule-molecule collision time is of the order of  $10^{-8}$  sec, which is the same order as the radiative lifetime of the singlet state ( $\tau \sim 48$  nsec at 3160 Å).<sup>7a</sup> Hence, the photochemical processes are most probably occurring through the relatively long-lived triplet state of HFA ( $\tau \sim 3.3$  msec).<sup>6</sup> It is to be noted that product I obtained by photolysis with *B*-trideuterioborazine has retained three deuterium atoms. This could indicate that an HFA intermediate has inserted into a B-H bond directly. The formation of II cannot be explained by a simple one-step process. Since abstraction of an H atom on the borazine ring occurs almost exclusively at the boron site, the following mechanism for the formation of I is proposed as an alternative to ring insertion

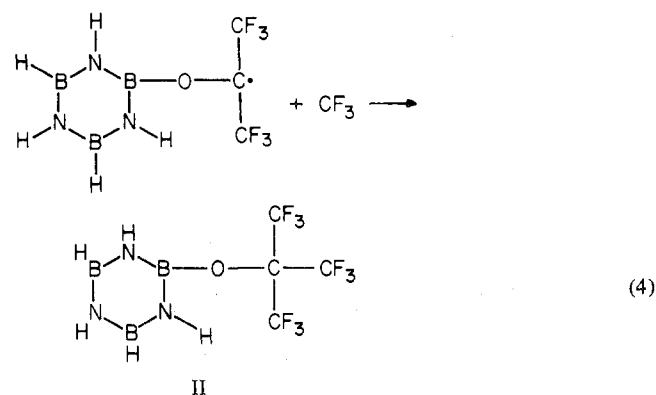
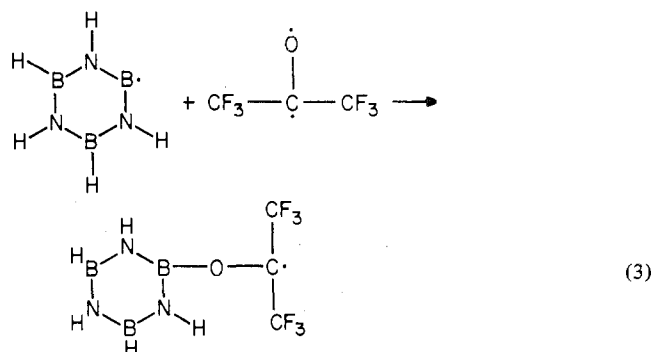


with radical recombination



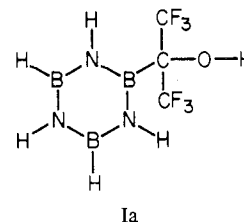
I

Similarly for product II radical recombination gives



II

Since product II is not formed directly from the photolysis of I with HFA, a process such as that indicated by eq 3 and 4 is necessary to explain the formation of II. There is no evidence in these studies for an isomer of I with structure Ia. This may



Ia

be contrasted with the photochemical reaction of HFA with cyclohexane<sup>17</sup> which leads to isomeric structures analogous to I and Ia. There appears to be little analogy between the photochemistry of HFA + benzene<sup>18-20</sup> and HFA + borazine since the former is controlled mainly by the chemistry of  $\text{CF}_3$  radicals. There was also no evidence in this study of any product with a structure involving substituent bonding at the N site. From the point of view of a free-radical mechanism this implies that the radical site of the boron atom is preferentially more stable than that at the nitrogen.

The infrared spectrum of II shows a large splitting of the N-H ring stretching frequencies. This effect, which is not observed for I, could result from a large electronic interaction of the  $(\text{CF}_3)_3\text{C-O}$  group with the borazine ring or from a structural change of the ring due to strong steric interactions.

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**Registry No.** I, 53431-88-2; II, 53431-89-3; borazine, 6569-51-3; HFA, 684-16-2; 2*H*-hexafluoro-2-propanol, 920-66-1; perfluoro-*tert*-butyl alcohol, 2378-02-1.

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### The Hexafluorobromine(VII) Cation, $\text{BrF}_6^+$ . Infrared Spectrum and Force Field

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The syntheses of  $\text{BrF}_6^+\text{AsF}_6^-$  and  $\text{BrF}_6^+\text{Sb}_2\text{F}_{11}^-$  from  $\text{BrF}_5$  and the corresponding  $\text{KrF}_2$  (Lewis acid) adducts have recently been reported by Gillespie and Schrobilgen.<sup>1,2</sup> These  $\text{BrF}_6^+$  salts were characterized by <sup>19</sup>F nmr and Raman spectroscopy.<sup>2</sup> Since complete vibrational spectra and modified valence force fields are known for  $\text{ClF}_6^+$ <sup>3</sup> and  $\text{IF}_6^+$ ,<sup>4-6</sup> similar information on  $\text{BrF}_6^+$  was desirable to obtain more quantitative data on the bonding in these unusual high oxidation state cations.

#### Experimental Section

**Apparatus and Materials.** The materials used in this work were manipulated in a well-passivated (with  $\text{ClF}_3$  and  $\text{BrF}_5$ ) 304 stainless steel vacuum line equipped with Teflon FEP U traps and 316 stainless steel bellows-seal valves (Hoke, Inc., 4251 F4Y). Pressures were measured with a Heise Bourdon tube type gauge (0–1500 mm  $\pm$  0.1%). Because of the rapid hydrolytic interaction with moisture, all materials were handled outside of the vacuum system in the dry nitrogen atmosphere of a glove box.

The infrared spectra were recorded on a Perkin-Elmer Model 457 spectrophotometer. The spectra of solids at room temperature were obtained by pressing two small single-crystal platelets of either  $\text{AgCl}$  or  $\text{AgBr}$  to a disk in a Wilks minipellet press. The powdered sample was placed between the platelets before starting the pressing operation. The low-temperature spectra were recorded at  $-196^\circ$  using a cell and transfer technique similar to one previously described.<sup>7</sup> The inner windows of the cell were  $\text{AgCl}$ ; the outer ones,  $\text{CsI}$  disks. The instrument was calibrated by comparison with standard calibration points.<sup>8</sup>

The Raman spectra were recorded on a Cary Model 83 spectrophotometer using the 4880-Å exciting line and a Claassen filter<sup>9</sup> for the elimination of plasma lines. For low-temperature work a Miller Harney device<sup>10</sup> was used. Passivated quartz, Teflon FEP, or Kel-F capillaries were used as sample tubes in the transverse-viewing, transverse-excitation technique.

Debye-Scherrer powder patterns were taken using a GE Model XRD-6 diffractometer with copper  $K\alpha$  radiation and a nickel filter. Samples were sealed in quartz capillaries ( $\sim 0.5$ -mm o.d.).

The purification of  $\text{BrF}_5$  and  $\text{AsF}_5$  and the preparation of  $\text{BrF}_5\cdot 2\text{SbF}_5$  have previously been described.<sup>11</sup> Krypton difluoride was prepared from Kr (Matheson, 99.995%) and  $\text{F}_2$  using glow discharge at  $-183^\circ$ . Our method was similar to that<sup>12</sup> of Schreiner, *et al.*, except for the elimination of the gas circulation system. The  $\text{KrF}_2$  was collected at the end of a run in a tared Teflon FEP U trap maintained at  $-78^\circ$ . The only detectable impurity in the  $\text{KrF}_2$  was a small amount of  $\text{N}_2\text{O}_5$  which could be removed by treatment of the crude  $\text{KrF}_2$  with  $\text{BF}_3$  at  $-78$  and  $-10^\circ$ , which converted the  $\text{N}_2\text{O}_5$  to nonvolatile  $\text{NO}_2+\text{BF}_4^-$ .<sup>13</sup> Pure  $\text{KrF}_2$  was obtained by pumping off the volatile material and trapping the  $\text{KrF}_2$  at  $-78^\circ$ .

**Preparation of  $\text{BrF}_6^+$  Salts.** The  $\text{BrF}_6^+\text{AsF}_6^-$  salt was prepared by the method of Gillespie and Schrobilgen<sup>2</sup> using a  $\text{KrF}_2:\text{AsF}_5$  mole ratio of 2:1 and a large excess of  $\text{BrF}_5$ . Complete material balances were obtained for the experiments. The yields of  $\text{BrF}_6^+\text{AsF}_6^-$  were found to range from 5.3 to 7.0 mol % based on  $\text{KrF}_2$  and the correct amounts of Kr and  $\text{F}_2$  were evolved.

For the synthesis of the  $\text{SbF}_5$  salt, weighed amounts of  $\text{BrF}_4^+\text{Sb}_2\text{F}_{11}^-$  were dissolved in  $\text{BrF}_5$ , and  $\text{KrF}_2$  was added at  $-196^\circ$ . The mixture was kept at  $25^\circ$  until no further gas evolution was observed. Volatile materials were removed at room temperature. The Raman spectrum of the solid residue was identical with that previously reported.<sup>2</sup> Since in a separate experiment we had demonstrated that  $\text{BrF}_4^+\text{Sb}_2\text{F}_{11}^-$  can be removed under a dynamic vacuum at  $50^\circ$ , this residue was warmed to  $50^\circ$  for 1 week under a dynamic vacuum. Starting originally with 1.02 mmol of  $\text{BrF}_4^+\text{Sb}_2\text{F}_{11}^-$  and 7.63 mmol of  $\text{KrF}_2$ , 23.2 mg of a white solid residue was obtained which according to its infrared and Raman spectra was mainly  $\text{BrF}_6^+\text{SbF}_6^- \cdot x\text{SbF}_5$  with  $x$  being less than 1.

#### Results and Discussion

**Synthesis and Properties.** The synthesis data are in excellent agreement with the reports<sup>2</sup> of Gillespie and Schrobilgen. The following observations deserve some comment. In the previous study<sup>2</sup> no material balances were obtained. In our study the yield of  $\text{BrF}_6^+\text{AsF}_6^-$  was found to be about 6 mol % based on the assumption that 1 mol of  $\text{KrF}_2$  could produce 1 mol of  $\text{BrF}_6^+$  salt. In addition, it was established that  $\text{BrF}_6^+\text{SbF}_6^- \cdot x\text{SbF}_5$  can be separated from  $\text{BrF}_4^+\text{Sb}_2\text{F}_{11}^-$  by vacuum sublimation. However, the resulting product was not of sufficient quantity and purity to allow further characterization and to determine whether the anion was mainly  $\text{SbF}_6^-$  or  $\text{Sb}_2\text{F}_{11}^-$ . When samples of  $\text{BrF}_6^+$  salts were placed in passivated quartz capillaries and flame sealed, Raman spectroscopy showed that at ambient temperature the  $\text{BrF}_6^+$  salts attacked the quartz with formation of the corresponding  $\text{O}_2^+$  salts. Similarly, the  $\text{BrF}_6^+$  salts interacted at ambient temperature with  $\text{AgCl}$ . The attack of  $\text{AgCl}$  by  $\text{BrF}_6^+\text{AsF}_6^-$  was much faster than that by the corresponding  $\text{SbF}_5$  salt and preempted the recording of  $\text{BrF}_6^+\text{AsF}_6^-$  infrared spectra at room temperature. In Teflon FEP containers the  $\text{BrF}_6^+$  salts were stored at room temperature for prolonged periods without noticeable decomposition.

**X-Ray Powder Data.** The observed and calculated X-ray powder diffraction data for  $\text{BrF}_6^+\text{AsF}_6^-$  are listed in Table I. The pattern was corrected for lines<sup>14</sup> due to  $\text{NO}_2+\text{AsF}_6^-$  resulting from the interaction<sup>13</sup> between  $\text{AsF}_5$  and some  $\text{N}_2\text{O}_5$  which was present as an impurity in the  $\text{KrF}_2$  starting material. The powder pattern of  $\text{BrF}_6^+\text{AsF}_6^-$  very closely resembles that<sup>4,15</sup> of  $\text{IF}_6^+\text{AsF}_6^-$  indicating that the two compounds are isomorphous. By analogy with  $\text{IF}_6^+\text{AsF}_6^-$ , it was indexed in the face-centered cubic system with  $a = 9.394$  Å. As expected, the unit cell of  $\text{BrF}_6^+\text{AsF}_6^-$  is slightly smaller than that of