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CRYSTAL STRUCTURES OF $[\text{Xe}_2\text{F}_3^+]$ $[\text{AsF}_6^-]$ AND $[\text{XeF}_5^+]$ $[\text{AsF}_6^-]$

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Publication Date

1973-09-01

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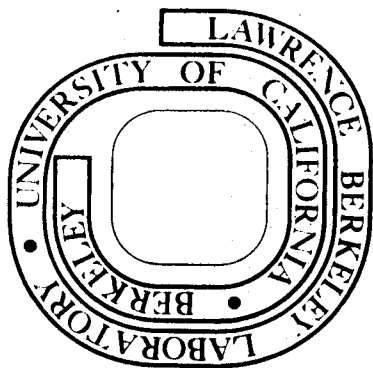
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September 1973

Prepared for the U. S. Atomic Energy Commission
under Contract W-7405-ENG-48

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LBL-1170

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Submitted to Inorganic Chemistry

LBL-1170

Contribution from the Divisions of Inorganic Materials Research and Nuclear Chemistry of the Lawrence Berkeley Laboratory and the Department of Chemistry, University of California, Berkeley, California 94720.

CRYSTAL STRUCTURES OF $[\text{Xe}_2\text{F}_3^+][\text{AsF}_6^-]$ and $[\text{XeF}_5^+][\text{AsF}_6^-]$

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D. H. Templeton and A. Zalkin

ABSTRACT

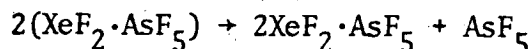
Crystals of $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$ are pale yellow-green. The crystalline modification which is stable at room temperature is monoclinic with $a = 15.443(10)$, $b = 8.678(5)$, $c = 20.888(15)$ Å, $\beta = 90.13(6)^\circ$, $V = 2799.3$ Å³, $Z = 12$, $d_c = 3.62$ gcm⁻³. The structure was refined in space group $I2/a$ using three-dimensional Zr-filtered Mo K α X-ray data. With anisotropic temperature factors for all atoms, a final conventional R factor of 0.048 was obtained for 1024 independent reflections for which $I \geq 3\sigma(I)$. The structure indicates the salt formulation $[\text{Xe}_2\text{F}_3^+][\text{AsF}_6^-]$. The structure analysis has not revealed any significant differences between the two crystallographically non-equivalent representatives of each ion in the asymmetric unit. The $[\text{AsF}_6^-]$ species are roughly octahedral, the 6 As-F distances being in the range 1.56(3) to 1.70(3) Å and the cis F-As-F bond angles in the range 83(2) to 95(2)°. The average As-F distance is 1.63(4) Å. The cation is V shaped $[\text{F-Xe-F-Xe-F}]^+$ and is planar and symmetrical about the bridging F atom. The average of the terminal Xe-F distances is 1.90(2) Å, the average bridging distance is 2.14(2) Å and the F(terminal)-Xe-F(bridge) angle is not significantly different from 180°. The average bridge Xe-F-Xe

angle is $150,2(8)^\circ$. Bonding in the cation can be represented by a resonance hybrid of the canonical forms $(F-Xe)^+ F^- (Xe-F)^+$, $F^- (Xe-F)^+ (Xe-F)^+$, and $(F-Xe)^+ (F-Xe)^+ F^-$, with the first form dominant.

Crystals of $[XeF_5^+][AsF_6^-]$ are colorless. The unit cell is monoclinic with $a = 5.886(3)$, $b = 16.564(10)$, $c = 8.051(4)$ Å, $\beta = 91.57(3)^\circ$, $V = 784.6$ Å³, $Z = 4$, $d_c = 3.51$ gcm⁻³. The structure was refined in space group $P2_1/c$ using three-dimensional graphite monochromatized MoK α X-ray data. With anisotropic temperature factors for all atoms a final conventional R factor was obtained of 0.12 for 925 independent reflections for which $I \geq \sigma(I)$. The asymmetric structural unit contains one XeF_5^+ and one AsF_6^- . Each cation makes F-bridging contacts to two anions (and vice versa) to define $(XeF_5AsF_6)_2$ centrosymmetric rings. Thus each cation is associated with one anion via a single F-bridge contact and with the other anion via a double F-bridge contact. These three bridging fluorine atom contacts with the cation are arranged approximately symmetrically about the pseudo-four-fold axis of the XeF_5^+ and below its basal plane. The XeF_5^+ has approximately C_{4v} symmetry, with the Xe-F axial distance = 1.78(2), the average Xe-F equatorial distance = 1.83(2) Å and the average F(axial)-Xe-F(equatorial) angle = $80(1)^\circ$. The AsF_6^- is somewhat distorted from O_h symmetry with bond lengths in the range 1.76(2) - 1.65(2) Å. The average As-F distance is 1.72(3) Å. The coordination of the cation is similar to that observed in the $[XeF_5^+]_2[AsF_6^{2-}]$ structure¹.

INTRODUCTION

Complexes of XeF_2 with AsF_5 were first reported by Bartlett and his coworkers². Initially they did not recognize that the 1:1 compound $\text{XeF}_2 \cdot \text{AsF}_5$ readily loses AsF_5 according to the equation:



and it was not until the crystal structure determination, reported in detail in this paper, was carried out that the compound first identified^{2a} with the composition $\text{XeF}_2 \cdot \text{AsF}_5$ was recognized as the salt $\text{Xe}_2\text{F}_3^+ \text{AsF}_6^-$. Although the compound $\text{XeF}_2 \cdot \text{AsF}_5$ has been established^{2b} and is thought to be $\text{XeF}^+ \text{AsF}_6^-$, crystallographic data to support that formulation is still lacking. Other $\text{Xe}_2\text{F}_3^+ \text{MF}_6^-$ salts were made subsequently^{2c} but the AsF_6^- salt remains the only one for which a structure determination is available.

Complexes of XeF_6 with F^- acceptors were discovered in three separate laboratories^{3,4,5}. The 1:1 complexes with AsF_5 and BF_3 were formulated on the basis of infrared evidence, by Bartlett *et al.*⁴, as XeF_5^+ salts. Although the crystal structure determination of $[\text{XeF}_5^+][\text{PtF}_6^-]$ (ref. 6) and its relative $[\text{XeF}_5^+][\text{RuF}_6^-]$ (ref. 7) gave firm structural support for the vibrational justification⁸ for $[\text{XeF}_5^+][\text{AsF}_6^-]$, it was clear from the powder data that this salt was not isostructural with its transition-metal analogues $\text{XeF}_5^+ \text{MF}_6^-$ ($\text{M} = \text{Ru}, \text{Rh}, \text{Os}, \text{Ir}, \text{Pt}$), in which series an isostructural relationship was assured⁷. It is usual for crystal structures of AsF_6^- salts to differ from those adopted by Sb and transition metal analogues⁹. It appeared probable that the coordination of the XeF_5^+ species in $\text{XeF}_5^+ \text{AsF}_6^-$ would differ from that observed in $\text{XeF}_5^+ \text{PtF}_6^-$ and $\text{XeF}_5^+ \text{RuF}_6^-$. Moreover, although the vibrational data provided strong circumstantial evidence for

the salt formulation, firmer evidence was desirable.

The formulation of the $\text{XeF}_6 \cdot \text{AsF}_5$ complex became a matter of greater interest when Bartlett and Sladky demonstrated¹⁰ that XeF_4 was a poorer fluoride donor than XeF_2 and would not form a complex with AsF_5 under ordinary temperatures and pressures.

EXPERIMENTAL

The 2:1 XeF_2 - AsF_5 complex was prepared as previously described^{2c}. Crystals of the compound (which is rapidly decomposed by water) were grown by sublimation under nitrogen (at ~ 1 atm) in sealed, dry, quartz X-ray capillaries, using the focused beam of a microscope lamp to heat the source material. The 1:1 XeF_6 - AsF_5 complex was prepared and single crystals were grown as described by Bartlett and Wechsberg⁸.

Crystal Data. - The selected crystal of F_9AsXe_2 (mol wt 508.5) was an approximate parallelepiped of approximate dimensions $0.1 \times 0.07 \times 0.05$ mm, the long edge being parallel with $\underline{b}$ and the other edges with $[101]$ and $[10\bar{1}]$. Precession and Weissenberg photographs established the lattice to be monoclinic and cell parameters were obtained from high angle measurements on an XRD5 diffractometer: $\underline{a} = 15.443(10)$, $\underline{b} = 8.678(5)$, $\underline{c} = 20.888(15)$ Å, $\underline{\beta} = 90.13(6)^\circ$, $\underline{V} = 2799.3$ Å³, $\underline{Z} = 12$, $\underline{d}_c = 3.62$ gcm⁻³. Observed reflections obeyed the relationships: $\underline{h} \ \underline{k} \ \underline{l}$: $\underline{h} + \underline{k} + \underline{l} = 2n$ and $\underline{h} \ 0 \ \underline{l}$: $\underline{h} + \underline{l} = 2n$, $\underline{h} = 2n$ ($\underline{l} = 2n$) and indicated the space group to be either $\underline{I}2/\underline{a}$ or $\underline{I}a$. (The space groups $\underline{I}2/\underline{a}$ and $\underline{I}a$ are unconventional representatives of $\underline{C}2/\underline{c}$ and $\underline{C}c$, respectively, which are the groups listed in International Tables¹¹.)

The selected crystal of F_{11}AsXe (mol wt 415.2) was a plate of approximate dimensions $0.28 \times 0.16 \times 0.04$ mm which was bounded by (001) , (010) ,

($\bar{1}01$), ($\bar{1}0\bar{1}$) and the capillary wall. The $\underline{b}$ axis was normal to the plate and approximately parallel to the axis of the capillary. Precession photographs established monoclinic symmetry and the systematic absences $\underline{h} \ 0 \ \underline{l}: \underline{l} \neq 2n$; $0\underline{k}0: \underline{k} \neq 2n$, indicated, uniquely, the space group $P2_1/c$ (No. 14)¹¹. Least-squares refinement of data from carefully centered high angle reflections gave: $\underline{a} = 5.886(3)$, $\underline{b} = 16.564(10)$, $\underline{c} = 8.051(4) \text{ \AA}$, $\underline{\beta} = 91.564(35)^\circ$, $\underline{V} = 784.6 \text{ \AA}^3$, $\underline{Z} = 4$, $\underline{d}_c = 3.51 \text{ g cm}^{-3}$.

X-Ray Measurements

F_9AsXe_2 .- Diffraction data were collected at room temperature ($24.5 \pm 1.5^\circ$) using Zr-filtered Mo $K\alpha$ radiation, $\lambda = 0.7107 \text{ \AA}$, with a manually operated single-crystal orienter on a G.E. diffractometer. The crystal was mounted with the $\underline{b}$ axis parallel to the ϕ axis of the orienter. Intensity measurements were made by the stationary-crystal stationary-counter technique, using a take off angle of 4° and 10 second counts. Backgrounds (also for 10 seconds) were measured at $2\theta \pm 1^\circ$ for reflections up to 30° and at $2\theta \pm 1.5^\circ$ beyond this point. Backgrounds were large. At small diffraction angles the background depended markedly upon 2θ and it was found to be more reliable, for such data, to obtain the background value from an empirical plot of background dependence on 2θ . Data for 1519 independent reflections were obtained, in the range $2\theta \leq 45^\circ$. Of these, 1024 met the criterion $I \geq 3\sigma(I)$. Several standard reflections were used to monitor the experiment at approximately 3 hour periods during the data collection. The standards showed no significant change in the course of data collection.

Correction for absorption ($\mu = 112 \text{ cm}^{-1}$) was made by the analytical method of DeMeulenaer and Tompa¹² using a program developed by Templeton and Templeton¹³. The usual corrections were made for Lorentz and

polarization effects and for anomalous dispersion.

F₁₁XeAs. - Diffraction data were collected at room temperature ($2\theta \pm 1^\circ$) on a Picker/Nuclear, four-circle diffractometer. Intensity data were collected with a θ - 2θ scan technique with Mo $K\alpha$ radiation, monochromatized with a graphite monochromator ($2\theta_m = 12.02^\circ$). A base width for the scan of 1.1° was used, which was centered on the predicted Mo $K\alpha_1$ position and was augmented on the high 2θ side to allow for the α_1 - α_2 separation. Each peak was scanned at a speed of $1^\circ/\text{min}$ and background measurements were counted for 10 seconds at each end of the scan. Attenuators were automatically inserted in the diffracted beam when the count rate exceeded 10,000 cps. Reflections were collected in the hemisphere $+\underline{h}$, $+\underline{k}$, $+\underline{l}$ for $2\theta = 0-50^\circ$ ($\sin\theta/\lambda = 0.596$). Three reflections were monitored periodically during the data collection and showed anisotropic deterioration from 43 and 63% of their original values. The data were corrected for this decay with a single (average value) function. A total of 1382 independent data were recorded of which 925 had $I > \sigma(I)$.

Because of the high X-ray absorption ($\mu = 90.8 \text{ cm}^{-1}$) and the large size and irregular shape of the crystal, an absorption correction was made by numerical integration. The correction varied by a factor 2.5 between extremes. Standard deviations of the intensities were calculated by $\sigma(I) = (\sigma^2(I_{\text{ave}}) + q^2 I^2)^{1/2}$, where q (here = 0.11) is a factor introduced to reduce the weights given to intense reflections, and $\sigma(I_{\text{ave}})$ was calculated from counting statistics or from the deviation of the individual reflections from the average, whichever was larger. Lorentz and polarization factors were then applied. For both structures atomic scattering factors for neutral F, Xe and As given by Doyle and Turner¹⁴ and the values of the dispersion corrections, for Xe and As, of Cromer and Liberman¹⁵ were used. Calculations were performed on our CDC 6600 and CDC 7600 computers¹⁶.

STRUCTURE DETERMINATIONS

F₉AsXe₂. - At the outset, the composition of the material was thought to be F₇AsXe, Z was assumed to be 16 and the space group was assumed to be I2/a. Study of the Patterson function revealed four sets of heavy atoms, each in the general position 8f. There was, however, some uncertainty as to which of xenon and arsenic should be assigned to the positions. Least-squares refinement, with all four eight-fold sets of heavy atoms assigned as xenon, proceeded to a conventional R factor of 0.24. The relative magnitudes of the thermal parameters indicated one of the atoms to be arsenic and a Fourier analysis revealed an additional heavy atom on the 2 fold axis (in 4d), the peak height of which indicated it to be arsenic. The Fourier analysis also showed 14 independent sites appropriate for F atoms. Full-matrix least-squares refinement, with all atoms assigned anisotropic thermal parameters resulted in a conventional R factor of 0.048 for 1024 independent non-zero data ($I \geq 3\sigma(I)$), with R (including zero weight data) = 0.091 for 1735 data. The weighted R factor (R_2) = 0.070. The g factor used was 0.08. The standard deviation of an observation of unit weight was 1.36. A difference Fourier revealed a number of small peaks (generally close to the heavy atom locations) all of which were $< 0.65 e \text{ \AA}^{-3}$. The atomic parameters from the last refinement are given in Table I. The observed structure factors, standard deviations and differences are given in the microfilm version of the paper in Table II.¹⁷

This analysis therefore established that the unit cell contained 24 Xe, 12 As and 108 F and thus revealed the composition of the complex to be $2\text{XeF}_2 \cdot \text{AsF}_5$; not $\text{XeF}_2 \cdot \text{AsF}_5$.

F₁₁AsXe. - Zachariasen's criterion¹⁸ of $18 \text{ \AA}^3$ per fluorine atom indicated that the number of formula units in the unit cell should be 4.

The three-dimensional Patterson function revealed the positions of the two heavy atoms in the asymmetric unit (each in general position 4e). Four cycles of least-squares refinement, with the atoms assigned isotropic thermal parameters brought the conventional R factor to 0.29. A subsequent electron density map revealed 11 additional major peaks which were designated as fluorine. Six of these were in an octahedral relationship to the As atom and five were in a square pyramidal arrangement about the xenon atom. Least-squares refinement proceeded initially with the thermal parameters isotropic for the F atoms and anisotropic for Xe and As; then all atoms were allowed anisotropic thermal parameters. An analysis of the weighted ΔF 's showed that the intense reflections had been given too much weight in the refinements, and that the parameter q in the standard deviation of an intensity needed adjustment. Values of q from 0.05 to 0.20 were tried, and $q = 0.11$ was chosen as best. Zero weight was assigned when $F^2 < \sigma(F^2)$. The final refinement yielded a conventional R factor of 0.12 for 925 reflections; including zero weighted reflections R = 0.14. The weighted R factor (R_2) = 0.13. The standard deviation of an observation of unit weight was 1.57. The shifts of all parameters were less than 2% of their estimated standard deviations. The final difference map showed smearing of electron density, about the Xe and As atoms, in the b direction; the peak heights were $7 \text{ e/\AA}^3$ near Xe and $4 \text{ e/\AA}^3$ near As. Other peaks were $2 \text{ e/\AA}^3$ or less.

These peaks and the high value chosen for q probably arise because of the pronounced intensity decay noted during data collection.

The atomic coordinates and thermal parameters are given in Table III and the structure factors, their standard deviations and final differences are given in Table IV¹⁷.

DESCRIPTIONS OF THE STRUCTURES

The atomic arrangements in the two structures are compatible with the salt formulations $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$ and $\text{XeF}_5^+\text{AsF}_6^-$. $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$.- The stereoscopic view given as Figure 1 shows the arrangement of the Xe_2F_3^+ and AsF_6^- ions within the unit cell¹⁹. There are two crystallographically non-equivalent ions of each type. The dimensions of the ions are detailed in Table V. The Xe_2F_3^+ ions are planar V shaped species and the two crystallographically distinct forms are not significantly different from one another. Each cation F-Xe-F-Xe-F is symmetrical about the bridging fluorine atom, the averaged Xe-F-Xe angle being $150.2(8)^\circ$ and each F-Xe-F component is essentially linear. The terminal Xe-F interatomic distances average to $1.90(3) \text{ \AA}$ whereas the bridging Xe-F distances average to $2.14(3) \text{ \AA}$. Figure 2 represents the averaged cation.

The interaction of the cations, one with another, as may be seen from Figure 1, generates a three dimensional network within the cavities of which the AsF_6^- ions are held. The network is a result of two short contacts of $\sim 3.0 \text{ \AA}$ each, involving interaction of the bridging F atom of one cation with one terminal fluorine atom on each of two other cations. Thus each bridging F atom of each cation is coordinated to 2 XeF groups, at $2.14 \text{ \AA}$, to define the cation, and two other F atoms (of two other cations)

at $\sim 3.0 \text{ \AA}$ to define the network. The plane, defined by the bridging F atom and the two close terminal F atoms at $\sim 3.0 \text{ \AA}$, is perpendicular to the plane defined by the cation containing the bridging F atom. The close atomic contacts of the bridging F atom are detailed in Table VI. Note that the alignment, of the bridging F atom, to the Xe-F groups at $2.14 \text{ \AA}$ and with each of the F-Xe groups at $\sim 3.0 \text{ \AA}$ is essentially linear. The arrangement of the two Xe atoms and the two F atoms about each bridging F atom can be viewed as grossly distorted tetrahedral. The next nearest atoms to the bridging F atom are F ligands of AsF_6^- ions, which are at distances of $3.4 \text{ \AA}$ or greater.

The departures of the anions in $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$ from octahedral symmetry are not statistically significant. Indeed the Raman spectrum of $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$ indicates^{2c} the anion to be close to the octahedral ideal whereas the spectrum of $\text{XeF}_5^+\text{AsF}_6^-$ (refs. 8 and 20) suggests a more distorted anion. $\text{XeF}_5^+\text{AsF}_6^-$. The atomic arrangement revealed by the structure analysis shows XeF_5 and AsF_6 groups which make close contacts to define the $(\text{XeF}_5\text{AsF}_6)_2$ rings shown in Figure 3. These rings have a form which is almost identical to that of the rings in the $(\text{XeF}_5)_2\text{PdF}_6$ structure¹. In this unit each XeF_5 group makes bridging contacts to two AsF_6 groups, via one F-ligand on one AsF_6 group and two F-ligands of the other. Three F-ligands (in cis relationship to one another) of each AsF_6 group each have bridging interaction with xenon. The intraionic distances and angles are listed in Table VII.

The XeF_5 group has essentially the same shape and size as the XeF_5 group in XeF_5PtF_6 (ref. 6), XeF_5RuF_6 (ref. 7), $(\text{XeF}_5)_2\text{PdF}_6$ (ref. 1) and in crystalline XeF_6 (ref. 21) and as in those cases is consistent with

designation as XeF_5^+ (see ref. 1). The AsF_6^- group, although distorted somewhat from the ideal octahedral symmetry of AsF_6^- , is nevertheless close enough in size and shape to be so designated. The average As-F distance is 1.72 Å with an average deviation of 0.03 Å. This is larger than the value for the $\text{Xe}_2\text{F}_{11}^+\text{AsF}_6^-$ case in which As-F = 1.63 Å with an average deviation of 0.04 Å. Evidently there is appreciable librational motion of the AsF_6^- species in the $\text{Xe}_2\text{F}_{11}^+\text{AsF}_6^-$ as indicated by the riding-motion-corrected As-F distances in this salt, which average to 1.74 Å with an average deviation of 0.03 Å. In $\text{XeF}_5^+\text{AsF}_6^-$ the As-F distance, corrected for libration, is 1.74 with an average deviation of 0.02.

DISCUSSION

These structures confirm that both xenon difluoride and xenon hexafluoride donate fluoride ion to generate the AsF_6^- ion. The discovery that XeF_2 and XeF_6 each form complexes with AsF_5 , but that XeF_4 does not, was made by Bartlett and Sladky¹⁰ and they exploited this finding to effect a chemical purification of XeF_4 . With AsF_5 , XeF_2 forms not only $\text{Xe}_2\text{F}_{11}^+\text{AsF}_6^-$ but also a 1:1 complex, which is presumably $\text{XeF}^+\text{AsF}_6^-$ (ref. 2) and XeF_6 forms $\text{XeF}_5^+\text{AsF}_6^-$ and $\text{Xe}_2\text{F}_{11}^+\text{AsF}_6^-$ (refs. 8 and 10), whereas XeF_4 does not form any complex under normal conditions of temperature and pressure. Evidently XeF_4 , as Bartlett and Sladky had supposed, must be an inferior F^- donor compared with either XeF_2 or XeF_6 . Only SbF_5 (which is the best F^- acceptor) forms XeF_3^+ salts^{22,23} with XeF_4 .

It is not, at first sight, surprising that XeF_4 is less effective than XeF_2 as a fluoride ion donor, since the greater positive charge²⁴ on the xenon atom in XeF_4 , relative to that for the XeF_2 case, is anticipated to

contribute to a greater ionization energy $[\Delta H, \text{XeF}_x \rightarrow (\text{XeF}_{x-1})^+ + \text{F}^-]$ for XeF_4 . Moreover, the greater size of the XeF_3^+ ion relative to XeF^+ , also renders the XeF_4 ionization less favorable than for XeF_2 . However, Berkowitz and his coworkers have determined²⁵ the ionization enthalpies for the xenon fluorides and although the XeF_4 ionization enthalpy is greater than for XeF_2 , it is only slightly so, the values being XeF_4 , 9.66 and XeF_2 , 9.45 eV. Presumably the ionization of XeF_4 is aided by a steric factor. If all non-bonding xenon electron pairs are visualized as being sterically active (which assumption is in accord with the observed stereochemistry²³), XeF_2 is a 5-coordinate, trigonal bipyramidal molecule and its simple ion XeF^+ is pseudo-tetrahedral. Xenon tetrafluoride is more crowded than XeF_2 , since it is pseudo-octahedral, hence conversion to the trigonal bipyramidal XeF_3^+ cation²³, may offer a more significant reduction in the ligand non-bonding pair repulsions than in the $\text{XeF}_2/\text{XeF}^+$ case.

The chemical evidence^{10,8} and the data²⁵ of Berkowitz and his coworkers, $[\Delta H, (\text{XeF}_6 \rightarrow \text{XeF}_5^+ + \text{F}^-) = 9.24 \text{ eV}]$ confirm that XeF_6 is the best fluoride ion donor of the xenon fluorides. In xenon hexafluoride, the ligand and non-bonding pair crowding is presumably much more severe than in the XeF_4 case. The seven coordinate molecule²⁶ generates a pseudo-octahedral cation on ionization. The evident steric activity of the non-bonding xenon valence electron pair in $\text{XeF}_5^+\text{AsF}_6^-$ again conforms to the pseudo-octahedral model, as Figures 3 and 4 demonstrate²⁷. There is, presumably, an appreciable decrease in the coordination sphere interactions accompanying the change $\text{XeF}_6 \rightarrow \text{XeF}_5^+ + \text{F}^-$ (ref. 28). This decrease in the ligand-ligand and ligand-non-bonding pair interactions must more than

offset those features which are less favorable to ionization in the XeF_6 case, i.e. (1) the greater charge on xenon in XeF_6 relative to XeF_4 or XeF_2 and (2) the greater size of the XeF_5^+ ion relative to XeF_3^+ or XeF^+ .

Xenon difluoride yields salts of the simple cation XeF^+ with the best fluoride ion acceptors and several salts of this cation have been described^{29,2,7} and its high electron affinity and its powerfully polarizing nature emphasized^{26,7}. The simple cation, however, readily combines with a second molecule of xenon difluoride to generate the Xe_2F_3^+ cation² which has been defined crystallographically in this study. The shape and dimensions of the Xe_2F_3^+ cation conform to its representation as a resonance hybrid of canonical forms $(\text{F-Xe})^+ \text{F}^- (\text{Xe-F})^+$, $\text{F}^- (\text{XeF})^+ (\text{Xe-F})^+$, and $(\text{F-Xe})^+ (\text{F-Xe})^+ \text{F}^-$, with the first form dominant. Indeed on this basis the salt $\text{Xe}_2\text{F}_3^+ \text{AsF}_6^-$ approximates to $(\text{XeF})_2^+ \text{F}^- \text{AsF}_6^-$. Fluoride ion is much more electron rich than any F^- ligand in AsF_6^- . It is, therefore, not surprising that the XeF^+ species should interact more strongly with F^- than with AsF_6^- , as the $\text{Xe}_2\text{F}_3^+ \text{AsF}_6^-$ structure, shown in Figure 2, demonstrates. It is of interest that recent work in these laboratories³⁰ has established XeF_2 complexes with PdF_4 (or PtF_4) of composition 2:1, 1:1 and 1:2, which Raman and infrared data indicate are $(\text{XeF})^+$ salts. There are also thermogravimetric data which suggest compounds $(\text{XeF}_2)_4 \cdot \text{PdF}_4$; these may well be $(\text{Xe}_2\text{F}_3)_2^+ \text{PdF}_6^{2-}$. Thus the Xe_2F_3^+ ion may even be stable in a doubly charged anion lattice.

The two fold coordination of the bridging F atom in Xe_2F_3^+ is reminiscent of the bridging F atom in F_3H_2^- (ref. 31). The relationship of the latter to F_4H_3^- and F_5H_2^- (ref. 32), poses the question of the

possible existence of the species $F_4Xe_2^{2+}$ and $F_5Xe_4^{3+}$. The dipositive cation may indeed be possible in the environment of a very favorable dinegative anion such as PdF_6^{2-} . The existence of a phase $(XeF_2)_3PdF_4$ has been indicated³⁰ but structural data are not yet available to settle whether the compound is $(Xe_3F_4)^{2+}PdF_6^{2-}$ or $(Xe_2F_3)^+ (XeF)^+ PdF_6^{2-}$.

Efforts to prepare the bridged species $Xe_2F_7^+$, by adding XeF_4 to $XeF_3^+SbF_6^-$ failed²³, but the bridged cation $Xe_2F_{11}^+$ has been recognized as a stable ion for several years⁸. Although crystals of $Xe_2F_{11}^+AsF_6^-$ have been grown from the melt and from bromine pentafluoride solution, and have provided unit cell and space group information⁸, no satisfactory crystal was found in our studies to warrant a structural study. Fortunately suitable single crystals of $Xe_2F_{11}^+AuF_6^-$ have been obtained and the structure is reported in the accompanying paper³³. Since the unit cell and space group of $XeF_5^+AuF_6^-$ (ref. 20) is the same as for $XeF_5^+AsF_6^-$ (indeed the salts are almost isodimensional) it is possible that the structure of $Xe_2F_{11}^+AsF_6^-$ will be similar to that seen in the gold compound.

The structure of $XeF_5^+AsF_6^-$ (Figures 3 and 4) is not like those of $XeF_5^+RuF_6^-$ (ref. 7) and $XeF_5^+PtF_6^-$ (ref. 6) in that each XeF_5^+ is coordinated to only 3 F atoms of two anions whereas in the other salts the cation is coordinated to 4 F ligands of four separate anions. Nevertheless, as has been discussed previously¹, the XeF_5^+ size and shape is not significantly different from that seen in the other XeF_5^+ salts (including XeF_6 itself). Moreover, the XeF_5^+ coordination in $(XeF_5)_2^+PdF_6^{2-}$ (ref. 1) is almost exactly the same as that seen here.

It is not yet known why certain octahedral anion salts (e.g. AsF_6^- , AuF_6^- , PdF_6^{2-}) should show different cation coordination than others

[e.g. RuF_6^- (ref. 7), PtF_6^- (ref. 6), IrF_6^- (ref. 10), SbF_6^- (ref. 34)]. The XeF_5^+ case is not an isolated one. It is usual for AsF_6^- salts of the alkali metals to be of NaCl type whereas for SbF_6^- , PtF_6^- , IrF_6^- , RuF_6^- the CsCl lattice is preferred⁹. Even $\text{IF}_6^+\text{AsF}_6^-$ has a NaCl lattice³⁵, whereas for $\text{IF}_6^+\text{MF}_6^-$ (M = Ru, Pt, Sb) a CsCl type is preferred³⁶. It seems that the coordinating character of the F ligand of AsF_6^- is not the same as for SbF_6^- , whereas the latter species appears to be similar to the majority of the transition metal MF_6^- . Certainly the AsF_6^- anion is smaller than the other MF_6^- mentioned. Also AuF_6^- is the smallest MF_6^- anion of the third transition series.³⁷ The structure type changes may, therefore, simply be related to the effective F ligand size although this in itself may be related to changes in the hybridization of the F ligand orbitals and the special arrangement of the formally non-bonding electrons of the F ligand.

ACKNOWLEDGMENTS

The work relating to $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$ was carried out during the tenure by one of us (N.B.) of a Miller Visiting Professorship (1967-68) and was also supported by the National Science Foundation under Contract No. GP-7153X. The remainder of the work was supported by the Atomic Energy Commission.

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16. The following programs were used in the solution of these structures: RLFACS, a program for reduction of raw data from the Picker automatic diffractometer; HORSE, our modification of Hamilton's GON09 program for absorption correction; INCOR and SORT, general data reduction programs; FORDAP, A. Zalkin's Fourier analysis program; LSLONG and LESQ, modifications of the Ganzel-Sparks-Trueblood least-squares program; DATLOK, D. J. St.Clair's unpublished weighting scheme analysis program; DISTAN and DISMAT, crystallographic bond distance and angle programs, the latter of which calculates standard deviations using the correlation matrix from least-squares; ORTEP, C. Johnson's (1965) thermal ellipsoid plotting program; LSPLAN, our modification of the least-squares planes program from the University of Pittsburgh; and LIST1 and LISTAP, data presentation programs.
17. A listing of observed and calculated structure factor amplitudes will appear immediately following these pages in the microfilm edition of this volume of the journal. Single copies may be obtained from the Business Operations Office, Books and Journals Division, American Chemical Society, 1155 Sixteenth Street, N.W., Washington, D.C. 20036. Remit check or money order for \$----- for photocopy or \$2.00 for microfiche, referring to code number INORT-00-0000.

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27. Note, in Figure 4, that the sites for the non-bonding pairs of the XeF_5^+ ions, which lie on the pseudo four-fold axes of the cations, are related by the center of symmetry of the $(\text{XeF}_5\text{AsF}_6)_2$ rings. The pseudo four-fold axis of one cation is tilted away from the other; this tilting would reduce the non-bonding non-bonding pair interactions.
28. There are a number of reasons for accepting the view that the bonding in the xenon fluorides maintains (approximately) the xenon octet whilst simultaneously satisfying the tendency of fluorine to adopt an octet (see, N. Bartlett, Endeavour, XXXI, 107 (1972)). Accordingly, each of the Xe-F bonds in the molecules (following J. Bilham and J. W. Linnett, Nature, 301, 1323 (1964)) is a single-electron bond whereas in a species such as Xe-F^+ the bond is an electron-pair bond. The formation of an electron pair bond must assist in the ionization process, $\text{XeF}_x \rightarrow (\text{XeF}_{x-1})^+ + \text{F}^-$, but this presumably would be approximately the same for each xenon fluoride. In the ionization of both XeF_2 and XeF_4 , separation of a linear F-Xe-F system into F^- and $(\text{Xe-F})^+$ occurs. Presumably, the separation of a fluoride ion from these fluorides is also assisted by the repulsive interactions of the F^- with the other ligand species and the non-bonding xenon valence electron pairs. Thus the XeF_2 molecule may be visualized as a trigonal bipyramid with three equatorial non-bonding "pairs". In the cation these three "pairs" have moved in toward the molecular axis along which the F^- has departed and they help shield the positive charge of the cation from the anion. Similarly, the removal of F, as F^- , from a corner of the square XeF_4 molecule, is visualized as being accompanied by a relocation of the two Xe "pairs" at the poles of

the molecule. This relocation brings the "pairs" towards one another (as they become equatorial "pairs" of the trigonal bipyramidal cation) and towards the departing F^- .

Although XeF_6 is not octahedral it is not far removed from that shape and we can allow that each F ligand has another F ligand at least approximately trans to it. In the ionization of XeF_6 , then, as in the other cases, we can assume that the removal of F^- is associated with the development of an electron pair Xe-F bond on the axis trans to it. But if we accept the structural evidence on XeF_5^+ as supportive of steric activity of the non-bonding Xe-valence-electron pair, the sterically active "pair" occupies the coordination site vacated by F^- . Perhaps, here, we have the major reason for the unexpected fluorobasicity of XeF_6 .

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TABLE I: Coordinates and Thermal Parameters for $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$ a, b, c

ATOM	X	Y	Z	B11	B22	B33	B12	B13	B23
XE(1)	-1379(1)	2975(2)	53644(9)	3.9(1)	4.0(1)	4.9(1)	44(8)	32(8)	-61(7)
XF(2)	-8486(1)	3047(2)	22164(9)	4.9(1)	3.03(8)	4.46(9)	-09(8)	09(8)	-37(7)
XE(3)	-8389(1)	3861(2)	11007(9)	4.1(1)	5.0(1)	4.6(1)	-81(8)	-37(8)	-49(8)
AS(1)	-4269(2)	7646(3)	4152(1)	5.3(2)	3.8(1)	4.7(2)	-2(1)	-3(1)	-21(1)
AS(2)	-250	250	250	4.1(3)	4.5(2)	4.5(2)	5(2)	-1(2)	-6(2)
F(1)	-250	361(3)	500	6.2(19)	7.0(17)	8.7(17)	0	2.9(14)	0
F(2)	041(1)	251(2)	6088(8)	6.5(13)	9.7(13)	5.3(9)	-1.3(10)	1.9(9)	-1.4(8)
F(3)	025(1)	-079(2)	2706(3)	7.5(13)	5.6(10)	6.6(10)	1.2(8)	-1.8(9)	-9(7)
F(4)	065(1)	192(2)	161(1)	6.3(15)	6.1(11)	16.3(19)	-9(9)	-3.8(14)	5.9(12)
F(5)	008(2)	561(2)	063(1)	9.2(17)	8.6(14)	11.7(16)	3.4(11)	2.1(13)	5.7(12)
F(6)	341(2)	705(3)	460(1)	10.1(21)	13.2(22)	14.2(20)	1.0(15)	6.8(17)	2.2(16)
F(7)	479(2)	607(3)	425(2)	13.2(26)	5.3(12)	20.1(36)	1.1(15)	3.8(26)	5.2(18)
F(8)	507(2)	815(4)	366(1)	11.2(23)	17.5(25)	9.5(15)	-5(18)	4.4(15)	4.2(15)
F(9)	366(2)	917(3)	397(2)	6.3(16)	7.9(15)	29.6(38)	1.5(12)	-3.0(21)	6.1(19)
F(10)	472(2)	952(4)	475(1)	10.3(32)	14.0(22)	13.5(21)	1.2(21)	-6.8(22)	-5.5(17)
F(11)	371(2)	678(4)	360(1)	19.1(34)	17.6(27)	9.5(17)	-7.1(24)	-3.9(19)	-4.4(17)
F(12)	152(2)	212(3)	243(2)	5.4(16)	12.3(20)	23.6(31)	-1.9(13)	-1.3(19)	-2.7(20)
F(13)	220(2)	324(4)	319(1)	9.1(22)	22.2(30)	11.3(10)	8.5(21)	-1.2(16)	-4.3(19)
F(14)	231(2)	409(4)	213(2)	10.6(23)	11.6(20)	29.2(37)	5.7(16)	1.7(23)	12.4(23)

a Estimated standard deviations of the least significant digit(s) are given in parentheses here and in tables III, V, and VI.

b The form of the temperature factor (B_{1j} in units of $\text{\AA}^2$) is: $T = \exp[-.25(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + 2B_{12}hk + 2B_{13}hl + 2B_{23}kl)]$.

c For space group I2/a the general positions are: $(x, y, z; \bar{x}, \bar{y}, \bar{z}; 1/2 + x, \bar{y}, z; 1/2 - x, y, \bar{z}) + (0, 0, 0; 1/2, 1/2, 1/2)$.

TABLE II: Observed Structure Factors, Standard Deviations, and Differences (x 2.0) for $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$

NOTE TO PRINTER: Table will be included only in the microfilm version of this paper.

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X 2.0) FOR
XE2F3.ASF6
F(0,0,0) = 2760

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K= 0, 0	8	191	8	4	-12	94	6	-12	2	258	11	-1	-15	48	14	7*			
2	0	11	-11*	10	158	7	-3	-10	454	19	-27	4	156	7	15	-13	135	7	5
4	68	4	17	12	143	7	12	-8	146	7	-4	6	254	11	1	-11	44	14	-5*
6	784	32	-76	14	149	7	-1	-6	203	9	-0	8	527	22	5	-9	148	7	1
8	97	5	37	16	24	32	1*	-4	498	20	-17	10	218	9	-2	-7	0	30	-2*
10	0	24	-3*	18	73	9	1	-2	120	5	2	12	97	6	13	-5	193	9	-0
12	104	6	-7	20	33	35	12*	0	92	4	10	14	301	13	-2	-3	72	8	3
14	32	16	30*	H,K= 0, 5	2	50	3	27	16	82	8	1	-1	290	12	13			
16	44	12	24*	1	335	14	18	4	396	16	-8	18	140	7	7	1	346	14	27
18	231	10	7	3	37	10	-16*	6	73	4	-9	20	61	11	6*	3	192	8	6
20	51	14	44*	5	100	6	16	8	268	11	16	H,K= 1, 4	5	206	9	-10			
22	38	25	36*	7	122	6	-4	10	167	7	-14	-19	83	9	4	7	159	7	4
H,K= 0, 1	9	38	12	35*	12	78	6	17	-17	35	23	17*	9	271	11	-0			
1	140	6	14	11	141	7	5	14	116	6	-0	-15	165	8	-0	11	36	17	29*
3	0	15	-3*	13	111	7	6	16	34	19	6*-13	41	13	12*	13	63	9	21	
5	511	21	3	15	0	32	-3*	18	0	32	-14*-11	21	28	16*	15	114	7	9	
7	274	11	-0	17	148	8	13	20	176	8	1	-9	36	12	-53*	17	87	9	2
9	51	6	-13	19	116	8	9	22	66	11	9	-7	297	12	-12	H,K= 1, 7			
11	233	10	-14	H,K= 0, 6	H,K= 1, 2	-5	49	7	-10	-14	92	8	-5						
13	238	10	9	0	244	10	6	-21	53	14	4*	-3	258	11	5	-12	90	8	11
15	58	9	27	2	71	7	5	-19	53	12	-9*	-1	242	10	20	-10	30	32	3*
17	23	32	4*	4	46	10	6*-17	123	7	-3	1	88	5	1	-8	68	9	-6	
19	0	33	-4*	6	230	10	12	-15	129	7	2	3	488	20	24	-6	225	10	-0
21	0	35	-7*	8	81	7	0	-13	20	28	0*	5	66	5	-13	-4	124	7	-8
H,K= 0, 2	10	76	8	5	-11	156	7	-3	7	169	7	-13	-2	78	9	2			
0	481	20	21	12	80	8	1	-9	88	5	-4	9	130	6	7	0	81	8	-4
2	516	21	36	14	43	15	21*	-7	150	7	-13	11	224	10	12	2	216	9	-15
4	202	8	-11	16	32	34	23*	-5	518	21	-7	13	108	6	9	4	154	7	-3
6	165	7	4	H,K= 0, 7	-3	109	5	-13	15	85	7	-8	6	135	7	3			
8	219	9	20	1	80	7	-8	-1	271	11	39	17	115	7	9	8	119	7	-6
10	217	9	-8	3	16	30	5*	1	528	22	58	19	18	34	2*	10	56	10	-2*
12	187	8	-30	5	48	12	11*	3	114	5	9	H,K= 1, 5	12	157	8	-0			
14	96	6	8	7	95	7	7	5	70	4	2	-18	19	35	3*	14	41	18	25*
16	162	8	-9	9	44	13	20*	7	158	7	0	-16	106	7	-9	H,K= 1, 8			
18	118	7	6	11	107	7	3	9	105	5	1	-14	102	7	-4	-11	53	13	11*
20	114	8	3	13	36	22	23*	11	61	6	13	-12	163	8	6	-9	52	13	7*
H,K= 0, 3	H,K= 0, 8	13	291	12	1	-10	278	12	7	-7	108	8	1						
1	112	5	4	0	0	32	-21*	15	64	8	6	-8	173	8	-0	-5	47	14	-6*
3	291	12	28	2	24	32	-18*	17	84	8	-0	-6	246	10	-13	-3	138	8	-3
5	26	12	2*	4	135	7	1	19	101	7	-7	-4	194	8	8	-1	176	9	5
7	31	10	11*	6	39	18	6*	21	53	14	8*	-2	0	28	-24*	1	0	32	-25*
9	467	19	-11	8	97	8	12	H,K= 1, 3	0	42	10	-4*	3	115	7	1			
11	65	6	6	10	91	8	-1	-20	32	35	6*	2	49	7	5	5	48	13	13*
13	36	14	12*	H,K= 0, 9	-18	101	8	-3	4	279	12	19	7	17	32	-2*			
15	127	7	-1	1	65	10	13	-16	73	8	-3	6	160	7	-3	9	31	33	8*
17	29	33	-29*	3	89	8	3	-14	85	7	15	8	0	27	-7*	11	115	8	8
19	18	33	6*	5	41	18	31*-12	102	6	-4	10	164	8	10	H,K= 1, 9				
21	63	12	5	H,K= 1, 1	-10	118	6	-0	12	131	7	5	-4	90	9	-9			
H,K= 0, 4	-22	73	10	8	-8	181	8	-3	14	68	9	-6	-2	0	37	-25*			
0	123	6	-6	-20	63	11	8	-6	204	9	-10	16	30	32	7*	0	59	13	-5*
2	114	6	9	-18	29	32	28*	-4	223	9	17	18	32	34	15*	2	88	8	7
4	298	12	17	-16	350	15	3	-2	103	5	6	H,K= 1, 6	4	72	9	-3			
6	191	8	-1	-14	184	8	5	0	438	18	28	-17	89	9	-5	H,K= 2, 0			

STRUCTURE FACTORS CONTINUED FOR
XE2F3.ASF6

PAGE 2

L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
-22	111	8	-14	20	44	16	21*	3	22	25	7*	1	90	8	2	-8	0	27	-19*
-20	195	9	9		H,K=	2,	3	5	91	6	6	3	36	23	24*	-6	411	17	-13
-18	30	33	1*-21	58	13	-2*	7	14	26-201*	5	85	8	8	-4	99	6	7		
0	90	4	-50	-19	82	9	10	9	57	8	-4		H,K=	3,	1	-2	166	8	12
4	523	21	-18	-17	108	7	7	11	133	7	-6	-22	53	16	5*	0	210	9	18
6	417	17	3	-15	90	7	-7	13	173	8	-7	-20	114	8	10	2	47	6	-1
8	306	13	-0	-13	235	10	-2	15	53	11	7*-18	109	8	2	4	151	7	11	
10	481	20	-20	-11	145	7	-6	17	59	11	10*-16	0	32	-20*	6	390	16	25	
12	161	7	8	-9	0	26	-15*		H,K=	2,	6	-14	140	7	-11	8	17	24	12*
14	340	14	3	-7	101	6	1	-16	0	34	-21*-12	208	9	-13	10	67	6	-3	
16	345	14	-1	-5	74	6	2	-14	97	8	-4	-10	155	7	-12	12	51	9	-8
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	H,K=	2,	1	3	173	7	3	-6	39	16	-2*	-2	656	27	39	20	18	34	10*
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-15	250	11	-16	11	86	6	1	2	61	8	16	6	132	6	-17	-15	30	34	-31*
-13	85	6	-3	13	43	11	1*	4	62	7	13	8	112	5	-12	-13	46	13	-6*
-11	90	6	8	15	95	7	3	6	29	22	19*	10	55	6	1	-11	118	7	-11
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-7	320	13	-16	19	59	11	-4*	10	119	7	-0	14	144	7	9	-7	221	10	3
-5	0	22	-2*	21	57	13	13*	12	29	31	25*	16	169	8	-13	-5	248	11	-10
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7	147	6	-5	-12	44	12	-2*	-9	70	9	2	-19	26	35	-8*	7	267	11	8
9	216	9	-11	-10	143	7	-12	-7	98	8	-8	-17	79	9	-15	9	52	8	6
11	159	7	-8	-8	153	7	11	-5	144	8	-0	-15	23	32	-15*	11	105	6	10
13	19	26	15*	-6	191	8	-11	-3	37	28	-9*-13	174	8	6	13	210	9	-1	
15	132	7	4	-4	126	6	5	-1	59	13	-14*-11	255	11	-2	15	48	12	9*	
17	42	14	13*	-2	396	16	33	1	0	31	-13*	-9	128	6	-12	17	94	7	-2
19	51	12	3*	0	188	8	9	3	68	8	-5	-7	281	12	1	19	55	12	8*
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-6	382	16	-3	20	70	10	2	-4	146	8	-8	13	56	8	13	-2	33	26	-12*
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4	754	31	-22	-13	122	7	-2	4	29	32	1*	21	37	24	5*	6	311	13	9
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8	131	6	5	-9	63	8	12	8	39	18	6*-20	43	20	-10*	10	123	7	-2	
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14	32	17	16*	-3	38	15	3*	-5	0	37	-22*-14	95	7	-7	16	25	32	15*	
16	49	11	3*	-1	222	10	2	-3	30	39	4*-12	520	21	-1	18	26	34	7*	
18	80	8	3	1	85	6	-6	-1	56	17	-10*-10	59	8	-14		H,K=	3,	6	

STRUCTURE FACTORS CONTINUED FOR
XE2F3.ASF6

PAGE 3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
-15	90	9	-5	18	112	7	14	-1	114	6	6	-4	239	11	12	10	163	7	1	
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-9	164	8	-10	-21	28	37	8*	5	90	5	6	2	201	9	9	16	53	11	5*	
-7	29	33	9*-19	99	8	19	7	50	7	-6	4	30	23	13*	18	51	12	12*		
-5	118	7	-11	-17	149	8	-1	9	272	11	112	6	40	13	14*	20	0	34	-9*	
-3	424	18	9	-15	95	8	-8	11	161	7	-7	8	47	12	-10*	H,K= 5, 2				
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1	62	8	-1	-11	84	7	-4	15	155	8	-13	12	17	31	-7*-17	136	8	-11		
3	182	8	19	-9	246	10	-10	17	0	31	-12*	14	25	33	20*-15	0	34	-13*		
5	186	8	-2	-7	163	7	-3	19	59	11	1*	16	0	34	-2*-13	102	7	-7		
7	34	17	11*	-5	302	13	11	H,K= 4, 4				H,K= 4, 7				-11	158	8	-4	
9	152	7	1	-3	142	7	-7	-18	0	36	-18*-13	62	12	7*	-9	248	11	14		
11	78	8	-5	-1	331	14	-4	-16	77	10	-10	-11	69	11	-6	-7	149	7	-6	
13	42	15	10*	1	472	19	1	-14	25	34	-22*	-9	109	8	1	-5	234	10	3	
15	203	9	0	3	93	5	-4	-12	0	32	-27*	-7	38	25	-8*	-3	230	10	-10	
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-12	33	35	-10*	9	209	9	-10	-6	35	19	-21*	-1	145	8	-13	3	0	22	-38*	
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-8	121	8	-12	13	111	6	1	-2	239	10	-7	3	37	19	-5*	7	259	11	-11	
-6	0	35	-21*	15	0	30	-36*	0	63	7	-1	5	95	7	-9	9	145	7	-8	
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14	45	16	23*-10	171	8	-7	H,K= 4, 5				5	-2	167	9	-0	-14	0	33	-3*	
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-7	44	20	-20*	-4	274	12	16	-13	129	8	-7	4	18	33	9*	-8	167	8	2	
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7	145	8	-0	10	29	15	4*	1	267	11	13	H,K= 5, 1				6	102	6	-3	
9	62	10	7	12	138	7	3	3	64	7	3	-20	52	16	6*	8	84	6	1	
H,K= 3, 9				14	341	14	4	5	300	13	1	-18	19	35	-2*	10	213	9	9	
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-2	49	22	28*	18	51	12	-23*	9	55	9	2	-14	325	14	1	14	130	7	-9	
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8	257	11	-7	-11	188	8	-5	-14	0	35	-14*	0	99	5	9	-15	122	8	5	
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12	259	11	-18	-7	180	8	5	-10	134	8	-11	4	216	9	-1	-11	51	13	1*	
14	32	17	9*	-5	72	7	-3	-8	44	17	-7*	6	0	22	-44*	-9	284	12	-1	
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STRUCTURE FACTORS CONTINUED FOR
XE2F3.ASF6

PAGE 4

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
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-1	0	28	-4*	8	48	13	5*	8	160	7	-5	1	300	13	-10	-4	472	19	14
1	38	11	6*	10	0	32	-5*	10	223	10	-18	3	80	7	2	-2	281	12	-11
3	325	13	-8	12	95	8	5	12	169	8	12	5	15	29	-3*	0	259	11	-21
5	30	15	-3*	H,K=	5,	8	14	113	7	2	7	26	29	21*	2	415	17	-8	
7	96	6	5	-9	42	27	-14*	16	0	31	-16*	9	0	30	-21*	4	218	9	-26
9	376	16	0	-7	68	14	5*	18	112	7	-3	11	74	8	5	6	223	9	-0
11	58	9	9	-5	136	9	13	20	0	34	-17*	13	156	8	5	8	208	9	14
13	103	7	-0	-3	0	39	-1*	H,K=	6,	3	15	43	16	11*	10	150	7	-9	
15	91	7	-3	-1	20	36	5*-19	0	38	-24*	17	45	16	-2*	12	0	29	-15*	
17	30	33	-10*	1	89	8	6	-17	39	26	-0*	H,K=	6,	6	14	27	31	5*	
19	32	35	3*	3	96	8	7	-15	156	8	-5	-14	20	38	-14*	16	74	8	-0
H,K=	5,	5	5	59	11	8*-13	80	9	-4	-12	0	38	-31*	18	47	14	1*		
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-2	37	19	-22*	16	0	31	-4*	3	371	15	8	4	121	7	-1	-9	34	28	-2*
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2	112	6	5	20	101	8	2	7	53	7	19	8	23	31	-19*	-5	262	11	4
4	20	28	-7*	H,K=	6,	1	9	155	7	2	10	63	10	2	-3	42	12	-27*	
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8	15	29	1*-17	53	15	-5*	13	58	9	-4	14	18	34	8*	1	18	26	6*	
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-13	108	8	-8	-1	414	17	-2	-14	116	8	-8	-1	0	35	-23*	15	59	10	-2
-11	138	8	-5	1	110	5	-6	-12	0	35	-29*	1	168	8	-5	17	74	9	-6
-9	27	36	-7*	3	0	22	-9*-10	172	8	-2	3	60	11	3	19	0	34	-3*	
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7	147	7	-3	19	44	16	12*	8	161	7	-7	-4	0	40	-17*	-6	331	14	21
9	74	8	-11	H,K=	6,	2	10	50	10	-6*	-2	45	21	-4*	-4	189	9	6	
11	250	11	-3	-20	0	38	-20*	12	111	7	-5	0	51	15	28*	-2	214	9	2
13	90	8	8	-18	87	10	5	14	59	10	-14	2	104	8	0	0	230	10	-7
15	57	12	-3*-16	26	36	-8*	16	0	33	-16*	4	80	9	1	2	30	16	4*	
H,K=	5,	7	-14	231	10	-1	18	0	34	-8*	6	61	8	2	4	59	7	2	
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-4	0	38	-26*	-4	150	7	11	-11	82	10	1	-16	39	28	8*	14	49	12	-8*
-2	159	8	-14	-2	30	18	-18*	-9	38	31	-14*-14	134	8	13	16	34	23	2*	
0	235	10	-12	0	38	11	14*	-7	158	8	7	-12	63	12	15*	18	115	8	8
2	34	25	2*	2	34	10	6*	-5	352	15	16	-10	181	9	-2	H,K=	7,	4	

STRUCTURE FACTORS CONTINUED FOR
XEZF3.ASF6

PAGE 5

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-17	46	21	-6*	0	26	35	22*	14	59	10	-15	H,K=	8,	6	-7	99	8	9	
-15	28	38	-7*	2	0	34	-16*	16	119	7	0	-12	0	39	-2*	-5	70	10	11
-13	214	10	3	4	61	10	-3	18	82	9	3	-10	36	39	-5*	-3	156	8	-11
-11	0	37	-39*	6	35	23	2*	H,K=	8,	3	-8	67	13	-16*	-1	143	7	-12	
-9	48	16	-16*	8	185	9	6	-17	21	39	-4*	-6	0	38	-8*	1	137	7	3
-7	156	8	-3	10	63	11	7	-15	41	28	-5*	-4	0	37	-2*	3	293	12	-10
-5	50	15	-13*	H,K=	7,	8	-13	0	37	-32*	-2	125	8	-10	5	199	9	-3	
-3	114	7	-8	-5	44	27	20*-11	53	15	6*	0	36	28	-9*	7	184	8	9	
-1	188	8	-5	-3	36	39	30*	-9	26	35	18*	2	0	33	-17*	9	0	30	-29*
1	194	9	1	-1	0	37	-11*	-7	204	9	17	4	89	8	-5	11	80	8	6
3	14	28	4*	1	19	36	-5*	-5	166	8	7	6	0	32	-20*	13	0	32	-22*
5	271	11	7	3	82	9	1	-3	105	7	-3	8	30	32	25*	15	90	8	-10
7	36	15	9*	5	105	8	4	-1	380	16	-17	10	0	33	-4*	17	26	34	-13*
9	103	7	-1	H,K=	8,	0	1	25	28	-2*	12	0	34	-2*	H,K=	9,	3		
11	77	8	-7	0	0	28	-11*	3	154	7	-2	H,K=	8,	7	-16	76	12	1	
13	50	12	-5*	12	103	7	-8	5	126	7	-2	-9	100	10	-0	-14	41	27	3*
15	90	8	5	14	32	26	-22*	7	90	6	4	-7	0	39	-1*	-12	28	37	16*
17	73	9	-9	16	123	7	16	9	56	9	-4	-5	0	39	-1*	-10	150	8	-2
H,K=	7,	5	18	26	34	-6*	11	113	7	-1	-3	110	9	-7	-8	154	8	-4	
-16	30	39	10*	H,K=	8,	1	13	85	8	-1	-1	64	12	10*	-6	263	11	-1	
-14	68	13	3*-19	22	40	21*	15	17	32	-13*	1	70	10	7	-4	39	20	16*	
-12	0	37	-2*-17	0	38	-22*	17	112	8	9	3	32	34	22*	-2	167	8	0	
-10	188	9	-1	-15	94	10	4	H,K=	8,	4	5	89	8	1	0	389	16	-4	
-8	46	19	-1*-13	0	37	-15*-16	21	39	19*	7	83	9	8	2	254	11	13		
-6	100	9	-9	-11	141	8	3	-14	129	9	-3	9	84	8	2	4	26	30	-9*
-4	318	13	-2	-9	174	8	20	-12	56	16	-12*	H,K=	8,	8	6	289	12	-3	
-2	192	9	-2	-7	24	33	11*-10	42	22	-3*	-4	44	27	32*	8	216	9	13	
0	123	7	4	-5	210	9	3	-8	26	36	1*	-2	154	9	-10	10	69	8	1
2	237	10	6	-3	385	16	12	-6	127	8	-2	0	35	37	15*	12	0	32	-45*
4	80	7	1	-1	108	6	-8	-4	104	8	-1	2	28	36	-1*	14	39	18	3*
6	49	11	3*	1	23	27	-7*	-2	109	7	-9	4	155	8	-8	16	26	34	-10*
8	0	31	-8*	3	171	8	8	0	27	31	3*	H,K=	9,	1	H,K=	9,	4		
10	51	11	-8*	5	93	6	-2	2	138	7	5	-18	0	40	-8*-15	42	28	9*	
12	24	32	-4*	7	194	8	-13	4	54	9	19	-16	36	39	27*-13	79	11	10	
14	66	10	2	9	130	7	1	6	123	7	11	-14	0	38	-14*-11	132	8	-1	
16	94	8	6	11	0	29	-32*	8	67	8	3	-12	90	10	3	-9	88	10	-12
H,K=	7,	6	13	140	7	-1	10	135	7	-6	-10	0	36	-19*	-7	110	8	-0	
-13	0	39	-27*	15	185	9	18	12	86	8	-1	-8	198	9	0	-5	32	36	14*
-11	107	9	3	17	0	33	-22*	14	0	32	-10*	-6	322	14	25	-3	223	10	-0
-9	139	8	-4	19	0	34	-9*	16	166	8	-2	-4	33	26	10*	-1	24	33	9*
-7	59	14	3*	H,K=	8,	2	H,K=	8,	5	-2	249	11	-11	1	172	8	8		
-5	0	38	-35*-18	99	10	5	-15	21	40	-4*	0	274	12	-1	3	74	8	-1	
-3	83	10	-15	-16	0	39	-35*-13	41	27	-10*	2	0	28	-11*	5	149	7	9	
-1	97	8	-3	-14	28	38	9*-11	158	9	-0	4	106	6	-9	7	106	7	-15	
1	97	8	-7	-12	201	9	6	-9	83	10	-24	6	168	8	8	9	51	12	-12*
3	258	11	-4	-10	69	10	6	-7	51	16	-12*	8	66	8	-0	11	90	8	-4
5	0	32	-31*	-8	69	10	24	-5	72	11	-17	10	255	11	1	13	43	16	-2*
7	136	7	-2	-6	116	7	12	-3	86	9	7	12	0	31	-16*	15	96	8	1
9	116	7	2	-4	239	10	4	-1	59	11	6*	14	41	16	-14*	H,K=	9,	5	
11	39	18	-6*	-2	0	29	-17*	1	170	8	8	16	159	8	-0	-14	30	39	25*
13	31	34	4*	0	240	10	7	3	32	25	11*	18	0	34	-12*-12	0	38	-16*	
H,K=	7,	7	2	259	11	1	5	156	8	13	H,K=	9,	2	-10	64	13	-11*		
-10	48	22	9*	4	239	10	-0	7	216	10	0	-17	83	11	13	-8	39	28	-7*
-8	75	12	-12	6	222	9	9	9	79	8	-6	-15	128	9	6	-6	44	23	-3*
-6	55	16	-4*	8	55	8	7	11	99	7	1	-13	125	9	9	-4	160	8	-9
-4	96	10	-8	10	300	13	8	13	77	9	-7	-11	128	8	4	-2	0	35	-9*
-2	137	8	3	12	0	30	-8*	15	0	34	-2*	-9	70	11	-3	0	46	15	-8*

STRUCTURE FACTORS CONTINUED FOR
XE2F3.ASF6

PAGE 6

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	67	10	-6	-10	181	9	5	5	0	33	-21*	13	144	8	3	0	0	34	-36*
4	91	8	-1	-8	143	8	4	7	94	8	-5	15	32	34	-6*	H,K= 12, 1			
6	190	9	0	-6	143	8	3	9	18	33	-2*	H,K= 11, 3				-15	111	10	11
8	45	14	-2*	-4	25	34	16*	11	51	13	16*-14	0	39	-2*-13	0	40	-9*		
10	95	8	-9	-2	212	9	3	13	53	14	-6*-12	77	11	12	-11	61	14	2*	
12	0	33	-166*	0	71	8	15	H,K= 10, 6				-10	96	10	1	-9	134	9	-5
14	61	11	10*	2	120	7	0	-10	0	39	-6*-8	20	38	-17*	-7	86	10	7	
H,K= 9, 6				4	31	24	20*	-8	47	22	2*-6	0	38	-19*	-5	27	38	-5*	
-11	0	39	-21*	6	27	30	2*	-6	36	39	3*-4	157	8	-10	-3	0	36	-13*	
-9	148	9	-6	8	0	30	-5*	-4	20	38	-8*-2	120	8	-8	-1	53	14	-3*	
-7	119	9	-15	10	79	8	-11	-2	39	26	-0*	0	88	8	-9	3	203	9	-4
-5	29	38	8*	12	0	31	-5*	0	73	10	7	2	0	32	-10*	5	0	33	-2*
-3	82	10	-6	14	121	7	-6	2	61	12	-5*	4	138	7	-11	7	56	11	-20*
-1	190	9	-15	16	55	13	-2*	4	66	11	24	6	77	8	-6	9	124	7	-3
1	107	8	3	H,K= 10, 3				6	68	10	-1	8	178	8	-2	11	64	10	9
3	81	8	-0	-15	47	22	-8*	8	88	8	-2	10	84	8	-16	13	36	24	11*
5	47	14	-10*-13	0	38	-34*	10	42	19	-7*	12	31	33	-5*	15	0	35	-17*	
7	87	8	8	-11	48	19	-10*	H,K= 10, 7				14	140	8	-1	H,K= 12, 2			
9	108	8	5	-9	168	9	-7	-5	49	22	11*	H,K= 11, 4				-14	57	17	6*
11	132	8	7	-7	0	37	-38*	-3	59	15	-10*-13	56	17	-9*-12	112	9	5		
H,K= 9, 7				-5	129	8	2	-1	40	25	28*-11	41	27	-9*-10	35	38	7*		
-8	81	12	11	-3	94	8	3	1	98	9	-3	-9	0	38	-22*	-8	103	9	-3
-6	147	9	2	-1	41	17	-17*	3	75	10	-4	-7	139	8	-5	-6	182	9	-1
-4	84	11	-2	1	43	14	12*	5	67	11	18	-5	0	38	-19*	-4	38	30	24*
-2	63	13	-3*	3	138	7	-1	H,K= 11, 1				-3	147	8	-10	-2	273	12	15
0	27	36	3*	5	87	7	9	-16	92	11	5	-1	63	12	-10*	0	95	8	-13
2	91	9	7	7	68	9	-0	-14	72	12	-0	1	0	34	-30*	2	0	33	-1*
4	0	35	-6*	9	183	8	-12	-12	137	9	7	3	153	8	-20	4	186	9	-12
6	88	9	-9	11	69	9	-9	-10	112	9	2	5	60	11	-10	6	0	33	-12*
8	38	23	15*	13	72	9	11	-8	0	37	-3*	7	0	33	-19*	8	0	33	-5*
H,K= 10, 0				15	66	10	-2	-6	91	9	-3	9	0	33	-7*	10	0	33	-13*
0	608	25	15	H,K= 10, 4				-4	57	13	-2*	11	103	8	9	12	18	34	-1*
14	148	8	-0	-14	87	11	-4	-2	234	10	8	13	45	16	14*	14	0	34	-15*
16	89	8	-8	-12	76	11	-4	0	102	7	7	H,K= 11, 5				H,K= 12, 3			
H,K= 10, 1				-10	77	11	0	2	51	12	-0*-10	76	12	2	-13	93	11	-26	
-17	37	40	17*	-8	141	8	-3	4	322	14	-7	-8	164	9	-5	-11	29	39	13*
-15	0	39	-9*	-6	128	8	-7	6	217	10	13	-6	71	12	2	-9	20	38	-8*
-13	144	9	5	-4	195	9	-7	8	0	31	-14*	-4	20	38	-15*	-7	40	29	-11*
-11	64	13	-8*	-2	18	35	-18*	10	183	8	-15	-2	115	8	-5	-5	0	38	-12*
-9	32	37	29*	0	59	11	5*	12	97	8	-4	0	0	35	-11*	-3	33	37	-18*
-7	247	11	13	2	210	9	-3	14	0	33	-18*	2	0	35	-32*	-1	153	8	5
-5	166	8	15	4	106	7	1	16	0	35	-30*	4	0	34	-23*	1	50	14	26*
-3	53	12	14*	6	0	32	-30*	H,K= 11, 2				6	60	11	-8*	3	0	34	-36*
-1	57	10	-12	8	37	19	-27*-15	0	39	-6*	8	51	13	11*	5	230	10	0	
1	49	11	-15*	10	107	7	4	-13	0	38	-2*	10	55	13	4*	7	0	33	-7*
3	52	10	7*	12	43	16	-0*-11	53	17	9*	H,K= 11, 6				9	53	12	13*	
5	269	11	4	14	37	24	12*	-9	64	13	-3*	-7	57	17	-2*	11	48	15	-5*
7	90	7	-1	H,K= 10, 5				-7	0	37	-7*	-5	99	10	-5	13	0	35	-4*
9	0	30	-2*-13	21	40	-1*	-5	264	12	0	-3	67	13	-6*	H,K= 12, 4				
11	217	10	7	-11	36	39	-15*	-3	43	18	-26*	-1	129	8	5	-12	52	20	-16*
13	84	8	-4	-9	0	38	-15*	-1	34	29	-12*	1	70	11	-5	-10	30	39	7*
15	31	33	-2*	-7	28	38	-11*	1	259	11	-1	3	0	35	-22*	-8	29	38	25*
17	26	34	9*	-5	122	9	-4	3	0	32	-17*	5	141	8	-5	-6	21	39	-6*
H,K= 10, 2				-3	139	8	-5	5	51	12	-14*	7	33	35	15*	-4	0	38	-22*
-16	168	9	10	-1	79	9	-11	7	0	31	-12*	H,K= 11, 7				-2	101	9	-2
-14	0	38	-9*	1	229	10	-1	9	81	8	-10	0	79	11	15	0	96	9	6
-12	115	9	0	3	132	8	-1	11	24	33	-10*	H,K= 12, 0				2	60	12	1*

STRUCTURE FACTORS CONTINUED FOR
XE2F3.ASF6

PAGE 7

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	148	8	-4	-2	67	12	-2	-3	73	12	-3	0	30	39	-8*				
6	0	34	-12*	0	0	36	-32*	-1	40	27	-15*	2	36	39	-4*				
8	60	11	14*	2	111	8	-0	1	78	10	-3								
10	88	8	-6	4	129	8	-5	3	43	20	-6*								
12	98	8	-1	6	110	8	3	5	64	12	11*								
	H,K= 12,	5		8	131	8	1	7	0	36	-9*								
-9	56	17	-2*	10	53	13	-1*	9	33	36	-6*								
-7	0	39	-24*	12	43	20	3*		H,K= 14,	4									
-5	140	9	-1		H,K= 13,	4	-6	49	22	-7*									
-3	49	16	-13*	-9	37	40	8*	-4	37	40	-11*								
-1	20	37	7*	-7	141	9	12	-2	148	9	2								
1	0	36	-4*	-5	95	10	1	0	28	38	-3*								
3	0	35	-14*	-3	28	38	-8*	2	0	37	-3*								
5	46	17	4*	-1	180	9	2	4	44	20	1*								
7	130	8	13	1	0	36	-18*	6	20	36	-3*								
9	95	8	6	3	0	35	-14*		H,K= 14,	5									
	H,K= 12,	6		5	42	20	1*	-1	30	39	5*								
-4	0	39	-8*	7	71	10	3	1	87	10	0								
-2	0	38	-7*	9	0	35	-2*		H,K= 15,	1									
0	60	14	9*		H,K= 13,	5	-8	152	9	10									
2	20	37	12*	-6	43	28	8*	-6	75	13	-1								
4	0	36	-21*	-4	52	19	11*	-4	0	39	-7*								
	H,K= 13,	1		-2	20	38	17*	-2	50	18	-2*								
-12	60	16	-5*	0	106	9	3	0	0	38	-6*								
-10	0	39	-19*	2	128	8	-2	2	0	37	-20*								
-8	46	22	-17*	4	34	36	14*	4	44	20	-7*								
-6	35	39	-2*	6	83	10	-6	6	128	8	10								
-4	0	38	-29*		H,K= 14,	0	8	20	36	2*									
-2	153	8	-3	0	106	9	18		H,K= 15,	2									
0	61	12	-12*		H,K= 14,	1	-7	31	40	8*									
2	103	8	1	-11	74	13	4	-5	30	40	0*								
4	59	12	-27*	-9	67	14	11*	-3	129	9	0								
6	0	34	-4*	-7	81	11	-2	-1	0	38	-5*								
8	103	8	-7	-5	0	39	-7*	1	137	8	2								
10	57	12	6*	-3	0	38	-24*	3	84	10	5								
12	89	9	2	-1	144	8	3	5	0	37	-14*								
	H,K= 13,	2		1	117	8	5	7	95	9	1								
-13	0	40	-22*	3	19	36	-12*		H,K= 15,	3									
-11	92	10	-3	5	19	35	-17*	-6	0	41	-20*								
-9	124	9	-2	9	50	15	-1*	-4	109	10	7								
-7	64	14	0*	11	74	10	1	-2	36	39	12*								
-5	0	38	-36*		H,K= 14,	2	0	20	38	-2*									
-3	47	19	-14*	-10	64	15	7*	2	141	8	5								
-1	49	16	-24*	-8	73	13	5	4	45	21	6*								
1	66	11	-12	-6	141	9	12	6	28	37	5*								
3	92	8	-8	-4	20	38	0*		H,K= 15,	4									
5	0	34	-37*	-2	52	16	2*	-1	0	39	-3*								
7	109	8	2	0	129	8	3	1	42	27	8*								
9	135	8	8	2	71	11	-11		H,K= 16,	1									
11	81	9	-4	4	33	36	5*	-5	0	41	-32*								
13	38	25	8*	6	19	35	-1*	-3	84	12	5								
	H,K= 13,	3		8	139	8	4	-1	87	11	4								
-12	143	9	12	10	33	36	12*	1	21	39	12*								
-10	21	39	1*		H,K= 14,	3	3	29	38	3*									
-8	41	27	-7*	-9	37	40	4*	5	103	9	10								
-6	128	9	10	-7	95	10	1		H,K= 16,	2									
-4	20	38	-2*	-5	30	39	-12*	-2	53	19	12*								

TABLE III
Coordinates and Thermal Parameters for $\text{XeF}_5^+\text{AsF}_6^-$.^a

ATOM	X	Y	Z	B11	B22	B33	B12	B13	B23
XE	.1957(3)	.1101(1)	.2501(2)	5.76(9)	8.41(11)	5.05(8)	.22(9)	.01(5)	.22(6)
AS	.6068(6)	.1067(2)	.7009(3)	4.16(15)	5.47(15)	3.03(12)	.07(15)	-.31(11)	-.43(10)
F1	.081(4)	.1888(10)	.126(2)	6.3(11)	6.6(9)	4.7(8)	.5(9)	.0(7)	1.2(7)
F2	.456(4)	.1590(11)	.187(2)	6.3(12)	7.6(11)	6.4(10)	-3.1(10)	1.6(9)	1.9(8)
F3	.179(4)	.0607(11)	.050(2)	6.4(11)	8.1(10)	3.6(7)	1.1(9)	-1.5(7)	-.8(7)
F4	-.109(3)	.0830(16)	.269(2)	3.5(9)	14.7(18)	5.3(9)	-2.5(11)	.4(7)	1.3(10)
F5	.161(4)	.1852(11)	.405(2)	7.4(13)	7.9(10)	4.4(8)	1.7(10)	-2.5(8)	-1.3(7)
F6	.474(4)	.0869(10)	.509(2)	7.7(12)	7.6(9)	2.9(6)	.2(9)	-2.7(7)	-.7(6)
F7	.377(3)	.1625(12)	.756(2)	3.9(9)	7.4(11)	7.1(10)	2.1(9)	1.2(8)	-1.3(7)
F8	.486(3)	.0176(11)	.772(2)	4.6(9)	7.0(9)	3.9(7)	-1.2(8)	-.0(6)	1.2(6)
F9	.834(3)	.0457(9)	.643(2)	3.8(8)	5.8(8)	5.7(9)	1.3(7)	1.5(7)	.6(7)
F10	.734(4)	.1875(10)	.620(3)	7.2(13)	5.9(9)	7.4(11)	-1.5(9)	1.0(10)	-.6(7)
F11	.741(4)	.1226(11)	.888(2)	8.1(13)	9.8(12)	2.8(7)	.7(10)	-2.0(8)	-1.9(7)

^a Thermal parameters as in Table I.

TABLE IV Observed Structure Factors, Standard Deviations, and Differences (x 1.0) for $\text{XeF}_5^+ \text{AsF}_6^-$

NOTE TO PRINTER: Table will be included only in the microfilm version of this paper.

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X 1.0) FOR
XEP5+ ASF6- F(0,0,0) = 742

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K= 0, 0	0	0	6	9	5	-2	H,K= 0, 11	0	34	5	8	6	8	0	1*				
2 393	23	78	7	29	2	2	1 20	1	3	0	-1*	7	41	3	6				
4 198	11	35	8	6	0	-0*	2 11	3	-1	2	33	2	8	8	5	4*			
6 118	7	19	9	11	5	1	3 0	0	-4*	3	5	0	5*	9	4	2*			
8 45	4	-3	H,K= 0, 6	4	33	2	3	H,K= 0, 19	H,K= 1, 3										
H,K= 0, 1	0	70	5	-19	5	13	2	1	6	0	4*	-9	14	5	-1				
1 34	2	2	1	48	3	-17	6	10	4	-4	2	4	0	3*	-8	32	3	-4	
2 88	5	15	2	55	3	-8	7	6	0	-8*	H,K= 1, 0	-7	42	3	4				
3 60	3	12	3	91	5	-14	H,K= 0, 12	-4	50	3	3	-6	44	3	3				
4 72	4	12	4	89	5	-7	0	30	4	2	-6	83	5	14	-5	55	4	6	
5 71	4	13	5	67	4	-4	1	18	1	2	-4	31	2	3	-4	59	4	-2	
6 37	2	6	6	22	2	-0	2	26	2	1	-2	11	2	1	-3	67	4	0	
7 16	2	3	7	65	4	8	3	29	2	4	0	69	4	17	-2	26	2	-1	
8 2	0	1*	8	7	0	-2*	4	3	0	1*	2	103	6	26	-1	132	8	-8	
9 10	4	2	9	37	2	-4	5	38	2	8	4	119	7	34	0	53	4	-1	
H,K= 0, 2	H,K= 0, 7	6	10	4	0	6	38	3	4	1	104	6	-14						
0 59	4	-24	1	23	1	-2	7	31	2	-3	8	20	3	0	2	89	5	-4	
1 69	4	-9	2	10	1	1	H,K= 0, 13	H,K= 1, 1	3	9	3	-1							
2 57	3	2	3	21	1	-1	1	12	2	-1	-9	22	2	1	4	180	10	11	
3 106	6	1	4	50	3	1	2	13	2	3	-9	30	3	3	5	16	2	0	
4 88	5	9	5	10	3	3	3	31	2	5	-7	61	4	9	6	128	9	19	
5 136	8	12	6	51	3	1	4	21	1	3	-6	39	2	8	7	33	3	2	
6 13	2	0	7	4	0	2*	5	15	2	-2	-5	125	7	25	8	55	4	-3	
7 105	6	19	8	15	2	-2	6	7	0	-2*	-4	57	3	7	9	3	0	-0*	
8 6	0	2*	H,K= 0, 8	7	2	0	-8*	-3	74	6	11	H,K= 1, 4							
9 56	3	-0	0	52	4	-12	H,K= 0, 14	-2	47	5	7	-9	0	0	-4*				
H,K= 0, 3	1	49	3	-9	0	96	8	16	-1	316	21	61	-8	32	4	-6			
1 16	1	-2	2	114	7	-13	1	15	3	1	0	96	6	17	-7	26	3	4	
2 51	3	-3	3	58	3	-2	2	75	4	13	1	216	12	35	-6	86	6	5	
3 8	2	2	4	84	5	-2	3	15	2	1	2	122	7	21	-5	16	2	-0	
4 46	3	2	5	51	3	1	4	30	2	-1	3	95	6	15	-4	64	4	-2	
5 30	2	4	6	37	2	2	5	16	2	-0	4	158	9	28	-3	53	3	-1	
6 62	4	8	7	41	3	-9	6	19	3	0	5	41	2	5	-2	11	2	-2	
7 31	2	4	8	12	4	-3	H,K= 0, 15	6	120	7	21	-1	24	2	-3				
8 11	3	5	H,K= 0, 9	1	7	5	-0	7	35	2	-1	0	32	3	-4				
9 0	0	-3*	1	17	1	-1	2	16	2	3	8	49	3	-0	1	70	4	-10	
H,K= 0, 4	2	20	1	-2	3	5	0	-6*	9	15	4	2	2	18	1	-3			
0 222	15	-90	3	32	2	2	4	14	2	1	H,K= 1, 2	3	74	4	0				
1 3	0	3*	4	11	3	-1	5	6	0	-5*	-9	3	0	1*	4	12	2	2	
2 187	11	-26	5	51	3	2	6	4	0	-2*	-9	10	0	8*	5	51	3	0	
3 57	3	-3	6	11	2	0	H,K= 0, 16	-7	6	0	0*	6	12	0	-1*				
4 142	8	2	7	18	2	-5	0	4	0	3*	-6	6	0	1*	7	3	0	-4*	
5 69	4	4	8	10	4	4	1	14	2	6	-5	14	5	4	8	20	4	-3	
6 70	4	5	H,K= 0, 10	2	7	0	0*	-4	41	3	6	9	1	0	1*				
7 33	2	2	0	102	7	-27	3	18	2	-3	35	4	2	H,K= 1, 5					
8 25	2	-5	1	4	0	-6*	4	4	0	-4*	-2	7	3	5	-9	24	7	-1	
9 22	2	-2	2	92	5	-4	5	24	2	3	-1	156	9	12	-8	19	2	3	
H,K= 0, 5	3	37	2	-6	H,K= 0, 17	0	17	1	216	13	4	-6	16	2	3				
1 14	1	-1	4	64	4	-0	1	2	0	1*	1	16	1	1	-5	151	9	1	
2 11	1	0	5	35	2	2	2	11	3	2	2	153	9	12	-4	12	5	-2	
3 52	3	-2	6	39	2	5	3	9	7	0	4	39	3	6	-3	170	10	-12	
4 41	2	-1	7	21	2	-2	4	13	2	1	5	130	8	16	-2	31	2	-5	
5 96	6	2	8	15	2	-0	H,K= 0, 18	5	130	8	16	-2	31	2	-5				

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF5- ASF6-

PAGE 2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-1	171	11	-28	0	40	5	1	4	63	4	4	0	21	2	8	-6	39	2	8
0	41	4	-5	1	63	4	-6	5	7	0	5	1	31	5	8	-5	46	6	7
1	101	6	-20	2	3	0	-4	6	42	5	-6	2	28	3	9	-4	54	4	12
2	90	5	-12	3	55	4	2	7	9	0	3	3	18	5	0	-3	40	3	6
3	117	7	-15	4	0	0	-5	H,K=	1, 12	4	0	4	28	4	0	-2	106	9	24
4	53	3	-4	5	35	2	1	-7	4	0	0	5	7	0	5	-1	10	6	-2
5	31	2	-5	6	13	3	-2	-6	0	0	-9	6	26	2	3	0	162	10	43
6	41	3	4	7	13	3	2	-5	6	0	-0	H,K=	1, 16	5	1	2	62	5	9
7	17	2	1	8	11	0	-3	-4	20	2	0	-5	7	0	5	2	37	2	1
8	17	2	-4	H,K=	1, 9	-3	-2	-3	6	0	-3	-4	4	0	3	3	34	3	8
9	5	0	-3	-8	0	0	-2	-2	12	3	-4	-3	3	0	-1	4	19	2	2
H,K=	1, 6	-7	35	5	-11	-1	-1	59	5	5	-2	-2	3	0	-1	5	68	6	8
-9	0	0	-4	-6	10	4	-1	0	20	2	-1	-1	13	4	0	6	30	3	0
-8	10	0	-6	-5	93	6	-2	1	69	6	4	0	13	3	1	7	50	4	8
-7	10	0	-4	-4	18	2	1	2	7	0	7	1	23	3	-0	8	2	0	0
-6	36	4	-1	-3	138	8	-12	3	56	3	3	2	4	0	0	9	36	2	-2
-5	13	3	-1	-2	22	2	2	4	3	0	0	3	22	2	-1	H,K=	2, 2	2	2
-4	58	3	-4	-1	123	9	-15	5	21	2	-4	4	3	0	-0	-9	18	3	2
-3	51	3	-4	0	5	0	-3	6	0	0	-1	5	11	5	-2	-8	6	0	-6
-2	48	3	-4	1	96	8	-7	7	12	4	3	H,K=	1, 17	-7	-7	9	0	1	
-1	82	5	-10	2	10	3	1	H,K=	1, 13	-4	0	0	0	0	-1	-6	31	2	2
0	13	2	-1	3	68	4	-5	-7	22	6	-2	-3	20	4	4	-5	47	4	0
1	28	2	-5	4	0	0	-5	-6	5	0	4	-2	4	0	3	-4	4	0	-2
2	54	3	-6	5	29	3	1	-5	35	4	-2	-1	22	5	2	-3	73	9	5
3	68	4	-3	6	14	2	0	-4	1	0	0	0	11	0	6	-2	10	2	1
4	6	0	-4	7	18	7	-3	-3	67	6	10	1	21	2	3	-1	98	6	6
5	56	3	2	8	9	0	-3	-2	4	0	1	2	18	2	4	0	0	0	1
6	19	2	0	H,K=	1, 10	-1	87	7	9	3	11	4	11	4	5	1	114	10	5
7	20	2	2	-8	16	4	-4	0	11	4	1	4	21	2	2	2	6	0	5
8	8	0	-1	-7	3	0	-0	1	78	9	11	H,K=	1, 18	3	200	18	14	4	
H,K=	1, 7	-6	25	4	0	-6	2	2	27	4	5	-3	4	0	3	4	7	0	4
-8	31	3	-4	-5	4	0	2	3	20	2	3	-2	5	0	4	5	162	15	16
-7	4	0	-2	-4	13	2	1	4	21	3	2	-1	0	0	-1	6	14	6	0
-6	28	3	0	-3	29	2	-0	5	14	2	3	0	3	0	-1	7	71	5	6
-5	10	4	2	-2	26	2	4	6	19	2	-1	1	0	0	-4	8	3	0	-4
-4	23	2	-4	-1	34	3	-2	7	13	5	2	2	0	0	-6	9	31	5	2
-3	22	2	-0	0	9	3	-2	H,K=	1, 14	3	7	0	7	0	-1	H,K=	2, 3	3	3
-2	24	2	-5	1	22	2	1	-6	16	2	-1	H,K=	1, 19	-9	-9	15	3	-0	
-1	23	2	-1	2	12	2	-1	-5	6	0	4	-2	9	0	5	-8	5	0	-0
0	39	4	-10	3	35	3	-0	-4	11	3	-1	-1	20	2	5	-7	36	6	7
1	23	2	-3	4	10	5	-2	-3	7	0	0	0	11	0	5	-6	41	7	5
2	105	6	-14	5	18	2	1	-2	9	0	-1	1	19	3	6	-5	30	5	1
3	22	2	-1	6	7	0	5	-1	0	0	-4	2	5	0	-2	-4	104	11	10
4	112	7	-6	7	0	0	-4	0	8	0	4	H,K=	2, 0	-3	31	12	1	5	
5	18	2	1	8	6	0	-3	1	3	0	0	-4	58	4	-3	-2	125	11	5
6	90	5	8	H,K=	1, 11	2	20	2	-0	-6	147	8	22	8	22	-1	43	3	0
7	3	0	-5	-7	10	0	3	3	10	3	4	-4	124	7	26	0	122	9	4
8	48	3	-9	-6	22	2	-1	4	6	0	-4	-3	132	8	23	1	6	0	-3
H,K=	1, 8	-5	24	2	2	0	5	2	2	0	-3	0	121	7	15	2	105	6	2
-8	15	5	-1	-4	29	2	-0	6	9	0	6	2	28	2	-1	3	21	3	3
-7	11	4	-6	-3	28	4	-2	H,K=	1, 15	4	30	2	4	4	5	4	78	5	3
-6	43	3	1	-2	33	2	-3	-6	12	4	2	6	31	2	4	5	47	6	4
-5	16	2	1	-1	40	3	-3	-5	21	4	2	8	27	3	5	6	33	3	1
-4	41	3	-3	0	29	4	0	-4	14	2	2	H,K=	2, 1	7	42	2	0	-2	
-3	18	2	-3	1	13	2	-1	-3	29	3	-0	-9	31	2	-1	8	23	2	1
-2	15	1	2	2	59	3	1	-2	20	2	7	-3	7	0	-3	9	23	2	4
-1	65	5	-7	3	2	0	-3	-1	35	3	8	-7	47	5	5	H,K=	2, 4		

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEP6- ASF6-

PAGE 3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-9	5	0	1*	-6	29	2	1	-2	67	4	-3	-6	24	18	-1	4	156	9	34
-8	43	4	-9	-5	33	2	-1	-1	41	4	0	-5	3	0	-3*	6	114	7	21
-7	4	0	-0*	-4	76	5	-7	0	31	2	-4	-4	32	7	-1	8	59	4	-1
-6	108	7	8	-3	25	2	-1	1	54	4	-1	-3	10	0	-1*	H,K=	3,	1	
-5	10	0	-2*	-2	143	9	-18	2	12	3	1	-2	39	3	7	-8	4	0	-3*
-4	132	8	6	-1	15	2	-4	3	53	3	-1	-1	7	0	1*	-7	48	3	-5
-3	16	2	1	0	116	10	-17	4	15	2	1	0	30	4	4	-6	7	0	-4*
-2	138	8	-3	1	7	0	3*	5	41	3	3	1	7	0	6*	-5	74	5	11
-1	112	7	9	2	102	6	-11	6	10	0	-0*	2	14	2	3	-4	61	4	11
0	89	7	-10	3	41	2	-2	7	17	7	-2	3	1	0	-3*	-3	46	3	7
1	42	2	-2	4	65	4	-2	H,K=	2,	11	4	5	0	0	3*	-2	69	4	14
2	56	3	-7	5	5	0	-2*	-7	6	0	-2*	5	8	0	3*	-1	26	3	-2
3	47	3	-3	6	18	2	2	-6	12	0	-3*	6	5	0	2*	0	44	3	9
4	3	0	-12*	7	0	0	-4*	-5	2	0	-3*	H,K=	2,	15	1	32	3	0	
5	50	4	0	8	2	0	1*	-4	35	2	1	-5	0	0	-6*	2	104	6	20
6	32	5	-3	H,K=	2,	8	-3	9	0	7*	-4	19	5	4	3	0	0	0	-8*
7	12	7	-3	-8	19	3	-7	-2	77	5	1	-3	2	0	-0*	4	83	6	15
8	21	4	-3	-7	10	0	6*	-1	9	0	1*	-2	22	6	1	5	26	3	2
H,K=	2,	5	-6	43	3	-2	0	94	9	5	-1	0	0	0	-4*	6	23	2	3
-8	8	0	-2*	-5	14	2	5	1	13	3	2	0	33	8	2	7	20	3	3
-7	27	2	-7	-4	65	4	-6	2	69	4	2	1	6	0	4*	8	13	4	7
-6	14	9	2	-3	15	2	-1	3	12	4	3	2	20	2	-1	H,K=	3,	2	
-5	37	3	-2	-2	60	4	-8	4	40	4	4	3	8	0	3*	-8	10	0	2*
-4	14	4	-3	-1	48	4	-8	5	14	4	-4	4	12	4	1	-7	56	4	-5
-3	7	0	-0*	0	35	3	-4	6	15	2	1	5	6	0	-3*	-6	11	5	1
-2	61	4	-5	1	69	6	-10	7	10	7	-1	H,K=	2,	16	-5	142	12	23	
-1	83	6	3	2	27	2	-1	H,K=	2,	12	-4	4	0	0	2*	-4	13	4	2
0	43	3	-2	3	67	4	-6	-7	0	0	-1*	-3	12	0	4*	-3	205	15	30
1	34	2	-4	4	10	5	-2	-6	8	0	-6*	-2	7	0	6*	-2	1	0	-0*
2	8	0	6*	5	49	4	2	-5	5	0	-1*	-1	10	0	-5*	-1	230	14	43
3	53	3	-2	6	15	2	2	-4	17	3	-0	0	6	0	-3*	0	74	4	16
4	0	0	-3*	7	22	2	-6	-3	29	2	1	1	25	7	4	1	157	9	21
5	59	3	2	8	15	3	-1	-2	22	2	1	2	2	0	-0*	2	57	3	7
6	5	0	1*	H,K=	2,	9	-1	38	4	3	3	3	29	6	3	3	40	2	2
7	35	2	-5	-8	5	0	3*	0	41	3	6	4	3	0	-3*	4	44	3	4
8	5	0	2*	-7	23	4	-7	1	67	6	4	H,K=	2,	17	5	48	3	4	
H,K=	2,	6	-6	2	0	-4*	2	17	2	3	-4	17	2	3	6	19	2	6	
-8	21	2	-4	-5	26	2	0	3	72	5	5	-3	1	0	0*	7	19	3	4
-7	12	4	-5	-4	9	0	4*	4	15	2	4	-2	20	3	3	8	14	5	0
-6	60	4	-1	-3	11	3	1	5	36	3	-8	-1	4	0	1*	H,K=	3,	3	
-5	9	0	-1*	-2	8	0	-2*	6	6	0	0*	0	19	2	5	-8	5	0	0*
-4	65	4	-4	-1	22	2	1	7	24	2	-4	1	10	6	6	-7	16	4	-3
-3	24	2	-4	0	32	3	-4	H,K=	2,	13	2	2	21	2	6	-6	4	0	-5*
-2	87	5	-5	1	10	3	4	-6	3	0	-3*	3	10	5	6	-5	37	3	5
-1	45	3	-9	2	13	3	-1	-5	10	9	3	H,K=	2,	18	-4	36	2	2	
0	46	4	-3	3	47	3	-1	-4	9	6	0	-2	14	9	3	-3	36	2	3
1	102	7	-11	4	10	5	3	-3	10	8	6	-1	0	0	-0*	-2	135	8	15
2	31	2	-4	5	37	3	4	-2	26	2	3	0	14	5	5	-1	5	0	-2*
3	113	7	-9	6	9	0	8*	-1	19	3	9	1	7	0	6*	0	138	11	13
4	6	0	-1*	7	27	3	-6	0	31	4	5	2	7	0	3*	1	15	2	2
5	79	5	-0	8	5	0	4*	1	5	0	1*	H,K=	3,	0	2	109	6	9	
6	0	0	-5*	H,K=	2,	10	2	2	27	2	3	-8	29	2	1	3	5	0	3*
7	34	2	-8	-7	11	4	2	3	12	3	2	-6	30	2	3	4	97	6	7
8	3	0	2*	-6	32	8	-9	4	10	5	-2	-4	58	3	10	5	12	5	1
H,K=	2,	7	-5	9	0	0*	5	16	3	-0	-2	80	5	11	6	38	2	2	
-8	11	0	1*	-4	62	4	-0	6	3	0	2*	0	194	11	35	7	20	2	-7
-7	10	0	-6*	-3	30	3	-2	H,K=	2,	14	2	2	120	7	25	8	13	5	4

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF5+ ASF6-

PAGE 4

L	FOR	SG	DEL	L	FOR	SG	DEL	L	FOR	SG	DEL	L	FOR	SG	DEL	L	FOR	SG	DEL
H,K=	3,	4	-6	7	0	-3*	3	20	8	-0	5	1	0	-6*	-2	9	0	4*	
-8	21	2	-0	-5	9	0	1*	4	59	6	1	H,K=	3,	15	-1	70	4	7	
-7	18	2	-3	-4	26	2	-0	5	9	0	2*	-4	10	0	2*	0	1	0	-0*
-6	25	2	-0	-3	11	4	-4	6	38	5	-6	-3	3	0	-2*	1	53	4	4*
-5	46	3	2	-2	76	9	-6	7	8	0	4*	-2	18	6	4	2	5	0	4*
-4	34	3	-1	-1	10	0	-3*	H,K=	3,	11	-1	4	0	-1*	3	33	9	-2	
-3	57	4	3	0	112	18	-12	-6	0	0	-2*	17	2	1	4	21	2	-0	
-2	18	2	-4	1	4	0	-0*	-5	5	0	-3*	1	0	-4*	5	6	0	1*	
-1	21	4	0	2	96	11	-12	-4	17	5	-1	2	20	2	1	6	9	0	2*
0	52	6	-7	3	0	0	-1*	-3	11	4	2	3	7	0	3*	7	16	4	-3
1	21	3	-1	4	63	4	-2	-2	33	7	-0	4	18	2	2	H,K=	4,	3	
2	89	7	-2	5	2	0	-2*	-1	7	0	-2*	H,K=	3,	16	-7	12	0	6*	
3	19	2	-2	6	22	6	-9	0	51	11	1	-3	31	6	4	-6	51	3	-7
4	99	6	3	7	8	0	-5*	1	8	0	3*	-2	8	0	4*	-5	22	3	1
5	17	2	-1	H,K=	3,	8	2	60	8	-2	-1	30	4	6	-4	94	9	7	
6	68	4	7	-7	23	5	-6	3	8	0	-4*	0	5	0	3*	-3	46	3	2
7	6	0	-2*	-6	15	3	-7	4	33	3	-7	1	24	2	7	-2	89	5	6
8	37	2	-9	-5	43	5	1	5	0	0	-1*	2	0	0	-1*	-1	49	3	3
H,K=	3,	5	-4	22	2	-0	6	16	3	-2	3	14	3	3	0	72	6	2	
-8	4	0	1*	-3	63	8	-3	H,K=	3,	12	H,K=	3,	17	1	60	7	4		
-7	32	4	-7	-2	18	2	-1	-6	12	4	5	-2	13	0	1*	2	20	2	-4
-6	5	0	-0*	-1	66	13	-7	-5	28	5	-8	-1	6	0	3*	3	64	8	6
-5	37	4	-1	0	21	3	-4	-4	0	0	-1*	0	19	3	5	4	37	5	-2
-4	25	2	-0	1	54	9	-7	-3	45	4	1	1	4	0	3*	5	41	3	4
-3	31	3	-1	2	74	10	-10	-2	5	0	-4*	2	14	7	4	6	23	2	-3
-2	9	0	3*	3	26	2	1	-1	50	14	3	H,K=	4,	0	7	17	11	-5	
-1	18	2	-2	4	55	5	-5	0	15	3	0	-8	11	0	1*	H,K=	4,	4	
0	2	0	-4*	5	13	3	2	1	35	5	1	-5	11	0	2*	-7	10	0	8*
1	10	6	3	6	25	8	-8	2	18	5	-3	-4	21	3	0	-6	12	6	10
2	29	3	-2	7	10	0	5*	3	10	6	-4	-2	56	3	2	-5	9	0	-5*
3	14	2	4	H,K=	3,	9	4	12	3	1	0	35	2	3	-4	16	3	-1	
4	14	3	1	-7	21	6	-4	5	9	0	6*	2	10	0	4*	-3	11	6	7
5	28	2	-2	-6	2	0	-3*	6	12	4	1	4	23	3	-2	-2	36	2	3
6	6	0	-0*	-5	29	3	3	H,K=	3,	13	6	14	9	1	-1	35	2	0	
7	23	2	-1	-4	9	0	2*	-6	1	0	-1*	H,K=	4,	1	0	23	2	-2	
8	5	0	2*	-3	28	6	2	-5	9	0	-6*	-8	23	2	0	1	6	0	2*
H,K=	3,	6	-2	11	4	9	-4	8	0	8*	-7	12	5	4	2	21	2	-3	
-8	13	3	1	-1	4	0	-4*	-3	2	0	-4*	-5	45	3	1	3	17	2	-0
-7	30	4	-6	0	11	3	4	-2	7	0	1*	-5	26	4	6	4	6	0	3*
-6	12	3	0	1	3	0	1*	-1	0	0	-3*	-4	74	5	8	5	0	0	-2*
-5	63	6	3	2	29	2	1	0	19	4	8	-3	38	4	7	6	19	6	0
-4	13	3	-2	3	4	0	-9*	1	4	0	0*	-2	68	4	7	7	5	0	-2*
-3	110	13	-2	4	0	0	-10*	2	21	7	-2	-1	104	6	15	H,K=	4,	5	
-2	13	2	4	5	6	0	-5*	3	6	0	1*	0	72	5	8	-7	16	5	0
-1	116	15	-10	6	4	0	2*	4	9	0	-3*	1	134	10	19	-6	12	0	3*
0	38	5	-2	7	19	2	-2	5	4	0	1*	2	38	4	7	-5	28	2	-2
1	75	10	-12	H,K=	3,	10	H,K=	3,	14	3	126	8	16	-4	13	3	4		
2	48	5	-5	-7	14	7	3	-5	3	0	0*	4	28	2	3	-3	42	4	-0
3	50	5	-7	-6	8	0	-3*	-4	6	0	3*	5	79	7	8	-2	22	5	1
4	60	4	-4	-5	16	2	-3	-3	0	0	-1*	6	24	2	-1	-1	79	5	-6
5	10	6	-9	-4	18	2	-0	-2	14	3	2	7	40	3	-2	0	19	2	-2
6	27	2	-4	-3	32	7	-1	-1	5	0	-1*	H,K=	4,	2	1	97	8	-16	
7	7	0	-3*	-2	25	2	1	0	18	4	1	-7	6	0	3*	2	26	2	-2
8	24	4	-4	-1	34	8	-1	1	6	0	3*	-6	7	0	3*	3	101	13	-15
H,K=	3,	7	0	27	4	-0	2	27	2	3	-5	31	4	1	4	8	0	3*	
-8	7	0	3*	1	17	7	1	3	3	0	1*	-4	8	0	3*	5	55	7	-14
-7	1	0	-2*	2	42	10	0	4	33	3	6	-1	76	5	7	6	5	0	-5*

OBSERVED STRUCTURES FACTORS (CONT) FOR
XE#5- ASF6-

PAGE 5

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	36	8	-4	3	63	10	-11	0	7	0	-4*	-1	0	0	-7*	2	18	3	-2
	H,K=	4,	6	4	12	4	8	1	3	0	1*	0	2	0	-2*	3	4	0	3*
-7	0	0	-2*	5	40	6	-9	2	1	0	-0*	1	13	4	-3	4	19	3	0
-6	4	0	4*	6	8	0	7*	3	13	4	7	2	26	2	1	5	0	0	-5*
-5	12	0	-5*	H,K=	4,	10		H,K=	4,	15	3	5	0	-2*	H,K=	5,	8		
-4	8	0	-7*	-6	5	0	4*	-3	4	0	-1*	4	23	3	-0	-5	18	6	-2
-3	35	3	-3	-5	4	0	4*	-2	16	5	0	5	7	0	3*	-4	24	3	1
-2	23	2	-3	-4	2	0	-4*	-1	15	6	2	6	25	3	-1	-3	13	5	-1
-1	45	3	-6	-3	12	10	3	0	15	7	5	H,K=	5,	4	-2	34	3	-3	
0	19	3	-1	-2	15	2	-2	1	22	4	4	-6	20	4	-2	-1	12	0	-3*
1	32	3	-11	-1	16	2	-3	2	9	0	4*	-5	15	0	-1*	0	37	7	-4
2	20	4	-1	0	6	0	-3*	H,K=	4,	16	-4	-4	43	4	-4	-1	6	0	-3*
3	15	3	-3	1	6	0	-4*	-1	16	3	-1	-3	22	2	1	2	33	5	-5
4	9	0	-5*	2	6	0	2*	0	10	0	7*	-2	72	12	1	3	7	0	-1*
5	7	0	-2*	3	0	0	-2*	1	8	0	-2*	-1	22	3	-2	4	24	7	-1
6	10	0	1*	4	7	0	-0*	H,K=	5,	0	0	0	81	10	-4	5	11	0	1*
7	0	0	-7*	5	3	0	1*	-6	28	3	0	1	2	0	-4*	H,K=	5,	9	
	H,K=	4,	7	6	10	0	-3*	-4	46	3	0	2	82	7	-3	-5	10	0	-7*
-7	4	0	1*	H,K=	4,	11	-2	74	4	6	3	3	0	0	-3*	-4	13	11	6
-6	38	2	-8	-5	0	0	-2*	0	98	6	3	4	47	5	-8	-3	21	3	-2
-5	0	0	-1*	-4	34	4	-7	2	121	7	21	5	17	4	1	-2	8	0	6*
-4	53	3	-2	-3	6	0	-5*	4	66	4	6	6	22	4	-6	-1	18	3	1
-3	2	0	-5*	-2	34	3	-6	6	37	4	9	H,K=	5,	5	5	0	7	0	4*
-2	62	4	-2	-1	11	3	-1	H,K=	5,	1	-4	0	0	0	-2*	1	3	0	2*
-1	5	0	4*	0	24	2	-1	-6	6	0	2*	-5	11	0	-8*	2	3	0	2*
0	41	3	-8	1	12	3	4	-5	23	3	5	-4	4	0	2*	3	0	0	-4*
1	11	5	-2	2	13	0	-3*	-4	10	0	-1*	-3	24	3	-1	4	0	0	-3*
2	23	2	-2	3	18	3	-1	-3	34	3	8	-2	0	0	-7*	H,K=	5,	10	
3	13	3	5	4	5	0	-3*	-2	7	0	-1*	-1	19	4	2	-4	23	3	-2
4	17	2	-4	5	16	5	2	-1	21	2	2	0	0	0	-8*	-3	22	3	-1
5	4	0	3*	H,K=	4,	12	0	0	0	0	-3*	1	9	0	-0*	-2	33	7	-4
6	18	3	-0	-5	15	6	3	1	9	0	2*	2	5	0	4*	-1	18	0	-2*
	H,K=	4,	8	-4	7	0	7*	2	10	0	2*	3	11	0	1*	0	31	6	-5
-7	0	0	-3*	-3	14	3	-4	3	20	3	-0	4	0	0	-2*	1	13	5	1
-6	0	0	-2*	-2	3	0	3*	4	24	8	8	5	13	0	-0*	2	33	7	-3
-5	7	0	-2*	-1	6	0	-4*	5	9	0	1*	6	0	0	-2*	3	12	0	-1*
-4	0	0	-1*	0	1	0	-1*	6	21	4	-2	H,K=	5,	6	4	24	2	2	
-3	13	5	0	1	16	2	-0	H,K=	5,	2	-6	12	0	1*	H,K=	5,	11		
-2	7	0	4*	2	11	0	0*	-6	8	0	3*	-5	25	3	-3	-4	14	4	1
-1	13	3	-3	3	9	0	-0*	-5	43	3	1	-4	16	5	-4	-3	10	0	3*
0	10	5	3	4	8	0	2*	-4	10	0	8*	-3	25	2	-4	-2	2	0	-7*
1	19	11	-7	5	6	0	1*	-3	36	2	5	-2	32	2	-2	-1	9	0	9*
2	6	0	2*	H,K=	4,	13	-2	7	0	0	2*	-1	18	5	-7	0	0	0	-1*
3	8	0	-3*	-4	11	6	-5	-1	30	2	3	0	35	2	-7	1	5	0	5*
4	12	9	6	-3	16	3	1	0	17	7	2	1	16	2	-4	2	7	0	1*
5	5	0	3*	-2	10	0	-3*	1	24	3	5	2	29	2	-7	3	5	0	4*
6	17	4	-8	-1	24	2	1	2	12	5	4	3	15	0	-5*	H,K=	5,	12	
	H,K=	4,	9	0	10	0	2*	3	33	2	6	4	20	6	-4	-3	16	6	3
-6	6	0	-0*	1	28	2	-3	4	5	0	-1*	5	23	3	-1	-2	12	0	3*
-5	12	5	-6	2	1	0	-6*	5	38	4	5	H,K=	5,	7	-1	7	0	-1*	
-4	0	0	-8*	3	30	2	1	6	13	0	10*	-5	0	0	-3*	0	13	6	-1
-3	30	2	-4	4	7	0	6*	H,K=	5,	3	-4	11	0	0	-5*	1	15	4	4
-2	5	0	2*	H,K=	4,	14	-6	6	0	0	-8*	-3	0	0	-0*	2	13	0	1*
-1	43	3	-4	-4	4	0	-1*	-5	13	0	4*	-2	3	0	-6*	3	13	0	2*
0	3	0	-4*	-3	4	0	2*	-4	12	0	-3*	-1	0	0	-4*	H,K=	5,	13	
1	55	6	-11	-2	12	4	-2	-3	11	9	2	0	4	0	2*	-2	7	0	2*
2	7	0	6*	-1	4	0	4*	-2	24	2	1	1	7	0	-4*	-1	7	0	-5*

OBSERVED STRUCTURES FACTORS (CONT) FOR
 XE⁹⁵ ASF6-

PAGE 6

[illegible]

TABLE V
Some Angles in $\text{Xe}_2\text{F}_3 \cdot \text{AsF}_6$

Atoms	Deg.	Atoms	Deg.
F-Xe-F-Xe-F^+ Ion		AsF_6^- Octahedron	
F(1)-Xe(1)-F(2)	177(2)	F(6)-As(1)-F(7)	94(2)
F(3)-Xe(2)-F(4)	179(1)	F(6)-As(1)-F(9)	86(2)
F(4)-Xe(3)-F(5)	176(2)	F(6)-As(1)-F(10)	94(2)
Xe(1)-F(1)-Xe(1)	150.3(8)	F(6)-As(1)-F(11)	80(2)
Xe(2)-F(4)-Xe(3)	150.0(6)	F(7)-As(1)-F(8)	86(2)
AsF_6^- Octahedron		F(7)-As(1)-F(10)	95(2)
F(12)-As(2)-F(13)	83(2)	F(7)-As(1)-F(11)	88(2)
F(12)-As(2)-F(14)	88(2)	F(8)-As(1)-F(9)	94(2)
F(13)-As(2)-F(14)	88(2)	F(8)-As(1)-F(10)	91(2)
		F(8)-As(1)-F(11)	95(2)
		F(9)-As(1)-F(10)	93(2)
		F(9)-As(1)-F(11)	85(2)
		F(6)-As(1)-F(8)	175(3)
		F(7)-As(1)-F(9)	173(3)
		F(10)-As(1)-F(11)	174(3)

TABLE V Continued

Interatomic Distances in $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$

Atoms	Dist(Å)		Atoms	Dist(Å)
F-Xe-F-Xe-F ⁺ ions				
Xe(1)-F(2)	1.93(2) ^(a)		F(6)-F(7)	2.41(4)
F(1)	2.14(1) ^(b)		F(9)	2.29(4)
Xe(2)-F(3)	1.87(2) ^(a)		F(10)	2.42(5)
F(4)	2.18(2) ^(b)		F(11)	2.15(4)
Xe(3)-F(5)	1.87(2) ^(a)		F(7)-F(8)	2.23(4)
F(4)	2.11(2) ^(b)		F(10)	2.37(4)
			F(11)	2.24(5)
AsF ₆ ⁻ octahedra ^{(c)(d)}				
As(1)-F(6)	1.70(3)	[1.79]	F(8)-F(9)	2.45(4)
F(7)	1.60(3)	[1.72]	F(10)	2.35(4)
F(8)	1.67(3)	[1.76]	F(11)	2.42(4)
F(9)	1.67(2)	[1.79]	F(9)-F(10)	2.37(4)
F(10)	1.61(3)	[1.73]	F(11)	2.22(4)
F(11)	1.63(3)	[1.75]		
			F(12)-F(13)	2.14(4)
As(2)-2F(12)	1.56(3)	[1.67]	F(13)	2.40(5)
2F(13)	1.65(3)	[1.76]	F(14)	2.20(4)
2F(14)	1.61(2)	[1.75]	F(14)	2.28(4)
			F(13)-F(14)	2.27(5)
			F(14)	2.34(5)

(a) Terminal fluorines. (b) Bridging fluorines.

(c) As(1) is in the general position; As(2) is on a center of symmetry.

(d) The thermal parameters (given in Table I) indicate

librational motion of the $[\text{AsF}_6^-]$ ion. The As-F distances

corrected for librational motion are given in square brackets.

TABLE VI

Coordination of the Bridging F Atom in the Xe_2F_3^+ Ion
(distances in Å, angles in Deg.)

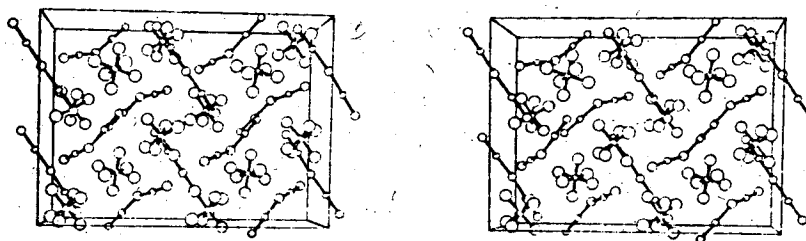
F(1) in F(2)-Xe(1)-F(1)-Xe(1)-F(2)		F(4) in F(3)-Xe(2)-F(4)-Xe(3)-F(5)	
F(1)-Xe(1)	2.14(1)	F(4)-Xe(2)	2.18(2)
		-Xe(3)	2.11(2)
F(1)-Xe(1)-F(2)	177(2)	F(4)-Xe(2)-F(3)	179(1)
		-Xe(3)-F(5)	176(2)
F(1)-F(5)	3.05(3)	F(4)-F(2)	2.98(3)
		-F(3)	3.03(3)
F(1)-F(5)-Xe(3)	173(1)	F(4)-F(2)-Xe(1)	153(1)
		-F(3)-Xe(2)	172(1)
F(1)-F(6)	3.41(4)	F(4)-F(13)	3.40(4)
F(1)-F(6)-As(1)	136(1)	F(4)-F(13)-As(2)	125(1)

TABLE VII
Interatomic Distances (Å) and Angles (Deg.)
Within the Asymmetric Structural Unit of $\text{XeF}_5^+\text{AsF}_6^-$
(Estimated standard deviations are, for all
values shown, 0.02 Å for distances and 1° for angles)

<u>Distances</u>		<u>Angles</u>			
Xe-F(1)	1.76	F(1)-Xe-F(2)	80	F(6)-As-F(7)	90
F(2)	1.82	F(3)	80	F(8)	87
F(3)	1.80	F(4)	82	F(9)	89
F(4)	1.86	F(5)	79	F(10)	90
F(5)	1.81	F(6)	141	F(7)-As-F(8)	92
F(6)	2.65	F(8) ^a	139	F(10)	92
F(8)	2.83	F(9) ^a	148	F(11)	92
F(9)	2.73	F(2)-Xe-F(3)	89	F(8)-As-F(9)	85
As-F(6)	1.74 [1.77] ^b	F(5)	89	F(11)	91
F(7)	1.71 [1.74]	F(3)-Xe-F(4)	86	F(9)-As-F(10)	90
F(8)	1.74 [1.75]	F(4)-Xe-F(5)	90	F(11)	89
F(9)	1.75 [1.77]	Xe-F(6)-As	158	F(10)-As-F(11)	91
F(10)	1.68 [1.71]	Xe-F(8)-As	110	F(6)-Xe-F(8)	63
F(11)	1.70 [1.73]	Xe-F(9)-As	114	F(9)	70
				F(8)-Xe-F(9)	50

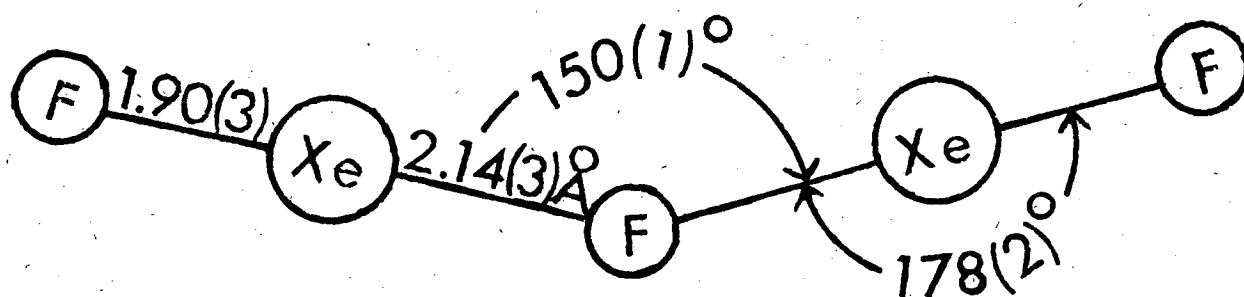
^a Atom related by center of symmetry at 1/2, 0, 1/2.

^b Values in square brackets are distances corrected for libration of the $[\text{AsF}_6^-]$ assuming riding motion of each light atom on the heavier.



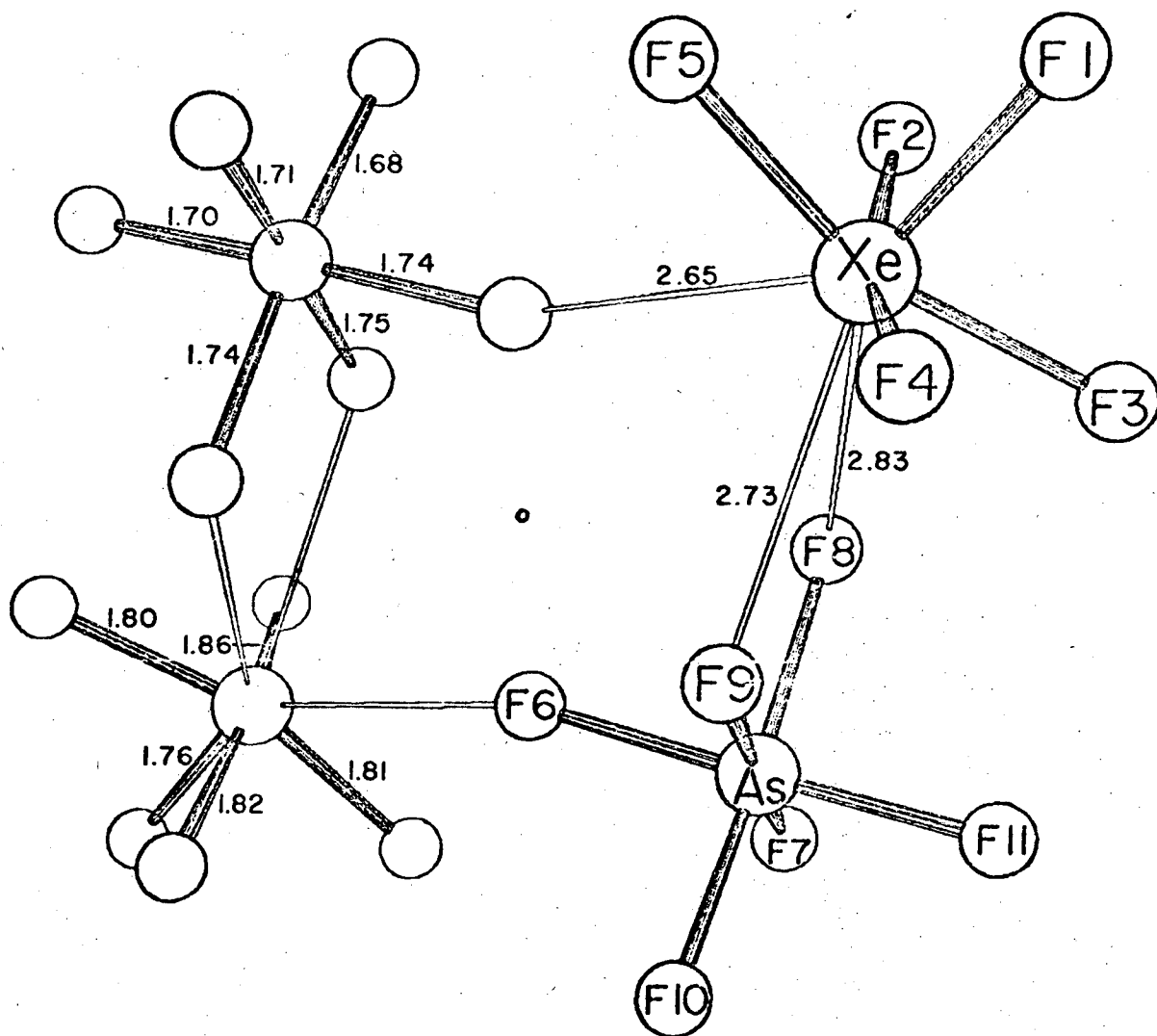
XBL 736-6315

Figure 1: Stereoscopic view of the $\text{Xe}_2\text{F}_3^+\text{AsF}_6^-$ unit cell, showing the arrangement of the ions (the unique axis, b, is normal to the plane of the paper and a vertical).



XBL 738-1120

Figure 2: The Xe_2F_3 Ion.



XBL 724-665

Figure 3: Configuration and bond distances for $\text{XeF}_5^+\text{AsF}_6^-$. Perspective view roughly perpendicular to the bc plane showing the cation-anion clusters about the center of symmetry at $1/2, 0, 1/2$. Estimated standard deviation for all bond lengths shown is $0.02 \text{ \AA}$.

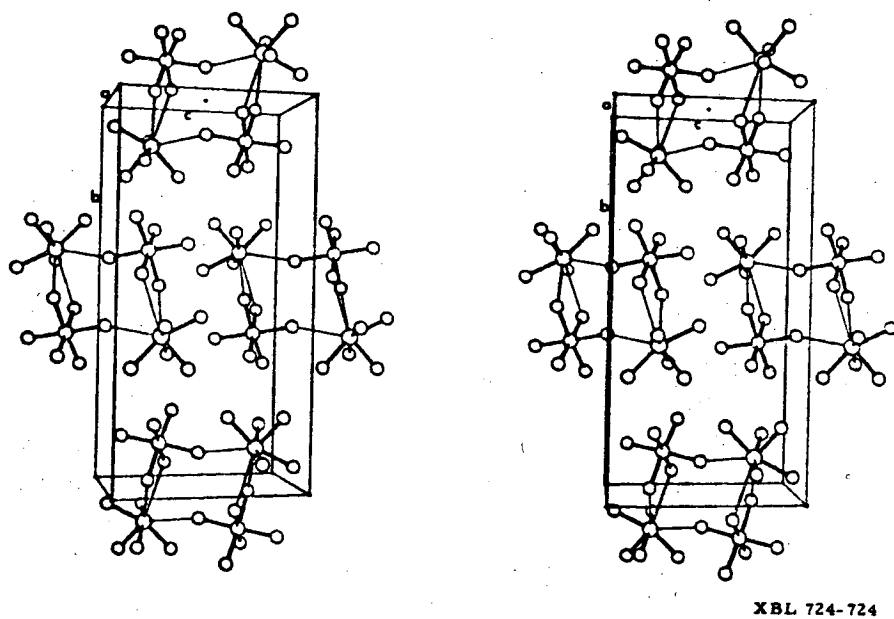


Figure 4: Stereoscopic view of the $\text{XeF}_5^+\text{AsF}_6^-$ structure.

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