Title
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by

D. McKee, A. Zalkin and N. Bartlett

Received:

ABSTRACT

Xenon tetrafluoride is a poor fluoride ion donor, forming complexes only with the strongest Lewis acid, antimony pentafluoride. The compound $XeF_4 \cdot 2SbF_5$ is triclinic with $\underline{a}$ = 8.237(5), $\underline{b}$ = 9.984(20), $\underline{c}$ = 8.004(5) Å, $\underline{\alpha}$ = 72.54(5), $\underline{\beta}$ = 112.59(7), $\underline{\gamma}$ = 117.05(21)°, $\underline{V}$ = 534.9 $Å^3$, $\underline{z}$ = 2, $\underline{d}_c$ = 3.98 gm cm^{-3}. Refinement has proceeded satisfactorily in space group $P\bar{1}$, using three dimensional graphite monochromatized MoK_α X-ray data. With anisotropic temperature factors for all atoms, a final conventional R factor of 0.035, for 1823 independent reflections, for which $I \geq 3\sigma(I)$, was obtained. The crystal structure contains discrete $XeF_4 \cdot 2SbF_5$ units and is consistant with the salt formulation, $XeF_3^+Sb_2F_{11}^-$. The T-shaped cation is planar; lying in the same plane as a forth fluorine atom, which makes a close contact of 2.50 Å to the xenon atom. This F atom, although part of the $Sb_2F_{11}^-$ ion, has a longer Sb-F bond of 1.90 Å. The other Sb-F bonds of the anion are in the range 1.84-1.86 Å. The xenon atom interacts with other fluorine atoms of the anion. The shape of the cation and the

nature of the interaction with the anions are consistant with a trigonal bipyramidal model for the cation, in which the two non-bonding valence electron pairs occupy equatorial sites.

EXPERIMENTAL SECTION

The 1:2 XeF_4-SbF_5 complex was made as described in the accompanying paper.[1] Crystals were grown by burying a Pyrex bulb containing a solution of XeF_4 in excess SbF_5, in a sand bath hot enough (~ 50°) to accomplish complete solution. The temperature of the bath was reduced over a two day period to room temperature. The SbF_5 was distilled at room temperature from the yellow crystals under dynamic vacuum to traps held at -196°. Pumping was continued for several days to thoroughly dry the crystals. A Raman spectrum of a conglomerate of crystals showed that they were the 1:2 compound[1].

CRYSTAL DATA

$XeF_4 \cdot 2SbF_5$ (mol. wt. 640.8) is triclinic with $\underline{a}$ = 8.237(5), $\underline{b}$ = 9.984(20), $\underline{c}$ = 8.004(5), $\underline{\alpha}$ = 72.54(5), $\underline{\beta}$ = 112.59(7), $\underline{\gamma}$ = 117.05(21)°, $\underline{V}$ = 534.9 $Å^3$, $\underline{z}$ = 2, $\underline{d}_c$ = 3.98 gm cm^{-3}, and F(000) = 559.86. Single crystal precession and Weissenberg photographs indicated that the space group is triclinic. A Delaunay reduction of the cell chosen, failed to show additional symmetry. The structure was successfully refined in the space group $P\bar{1}$.

X-RAY MEASUREMENTS

A clear, roughly cubic crystal of edge 0.10 to 0.15 mm was chosen for data collection. A Picker automatic four circle diffractometer,

equipped with a fine focus Mo anode tube, was used. High angle reflections were accurately centered at a take off angle of ~ 2° and were used for a least-squared refinement of the cell parameters. Data were collected and treated as described in a recent article[2]. A complete hemisphere of data was collected for $2\theta \leq 55°$. Intensities of three standards were collected at intervals of every 200 reflections. A total of 2662 intensity data were recorded.

STRUCTURE REFINEMENTS

The least-squares program used in the structure refinements has been described[2]. Scattering factors for neutral fluorine, xenon, and antimony were used as given by Doyle and Turner[3]. Anamolous dispersion factors were given by Cromer and Liberman[4].

Since the intensities of the standards were observed to diminish (finally to 85% of their original values) in a regular and nearly isotropic manner, the data were scaled linearly between each pair of standards. Associated with this decrease we also noted a decrease in the parameters b and γ (which were in the end reduced by .02 Å and .21° from their initial values). Broadening of the omega scans of the standards from .10 to .35° was also observed. The positions of the heavy atoms were determined from a three dimensional Patterson synthesis. These positions were subjected to least-squares refinement as xenon atoms, after which it was possible to separate the antimony atoms by exploiting temperature factor differences. The positions were then further refined. A difference Fourier revealed positions for 12 of the 14 fluorine atoms. Least-squares refinement of these positions was followed by another difference Fourier which revealed the positions of the final two fluorine atoms. Refinement of all these

positions, with anisotropic temperature factors, resulted in a conventional R factor of .06.

Examination of the observed and calculated structure factors showed that the poorest agreement occurred with the low angle, high intensity reflections. Since absorption and extinction corrections could not be reliably made, the lower angle data ($\sin\theta/\lambda \leq .32$) were given zero weight in the final least-squares refinements. This proceedure resulted in $R = 0.035$, $R_2 = .03$, and a standard deviation for an observation of unit weight of 3.7. The number of non-zero weighted data in this refinement was 1823. The positional and thermal parameters, reported in Table I, are from this refinement. Observed structure factors, standard deviations and differences in Table II are given in the microfilm version of this paper.[5] The highest peak on a final difference Fourier proved to be only 2 $e/\mathring{A}^3$. Table III gives chemically significant distances and angles.

DESCRIPTION OF STRUCTURE

The xenon atom is close-coordinated to three F atoms which define an approximately T-shaped species. The remaining atoms define an Sb_2F_{11} unit which consists of two approximately octahedral SbF_6 groups, sharing a common F atom, such that the angle Sb(1)-F-Sb(2) is 155.4(2)°. The bridging Sb-F interatomic distances (average distance - 2.02 Å) are significantly longer than the non-bridging, with the exception of that F atom (F(2)) which makes a close approach, of 2.50(1) Å, to the Xe atom. The interatomic Sb-F(2) distance is 1.90(1) Å. It is of interest that the F atom which makes this close approach to the Xe atom, is in cis relationship to the F atom of the Sb(1)-F-Sb(2) bridge.

The Sb_2F_{11} species seen in this structure is similar to those previously reported[6,7], but the XeF_3 species is novel. Only the bridging Sb-F distances differ significantly from 1.85 Å.

As Figure 3 illustrates, all four atoms of the XeF_3 species are in the same plane, but, furthermore, the F(2) atom of the Sb_2F_{11} unit, which makes the close approach of 2.50 Å to the Xe atom, is also in the same plane. Three other Xe contacts, to F(13), F(3) and F(7), of 2.94(1), 2.97(1), and 3.04(1), respectively, are made between formula units, as may be discerned from the stereogram given as Figure 2, in conjunction with Figure 1a.

DISCUSSION

The observed structure is consistent with the salt formulation $XeF_3^+ Sb_2F_{11}^-$. Other Sb_2F_{11} salts reported[6,7] hithertoo are $XeF^+Sb_2F_{11}^-$ and $BrF_4^+Sb_2F_{11}^-$. The $Sb_2F_{11}^-$ ion geometry has been discussed by Lind and Christe[6]. The former salt is also of interest in that it defines the Xe(II) cation XeF^+.

Although the short in-plane contact of 2.50(1) Å between the XeF_3^+ ion and the closest F atom (F(2)) of an anion could be represented as an indication of some covalency, the ionic model provides a simple and direct accounting for the observed structural features, if due allowance is made for the polarizing character of the cation.

No matter which bonding model we use for the XeF_3^+ cation[8], we conclude that two non-bonding valence-electron pairs of the xenon atom are not involved in bonding. If we allow the two non-bonding valence-electron pairs to be sterically active then they will, with the three

F-ligands, constitute a five coordinate arrangement for the xenon atom. As with the majority of five-coordinate non-transition element compounds, we might therefore expect the geometry to be based on a trigonal bipyramid[9]. Since the species ClF_3^+ and BrF_3^+ (which are electronically related to XeF_3^+) are T-shaped[10,11], we could therefore anticipate that the XeF_3^+ non-bonding pairs would be in the equatorial plane as illustrated in Figure 4. Such a cation would be far from spherical in its polarizing effect on anions. Indeed, the screening effects and replusive effects of the non-bonding electron pairs and the F-ligands should result in a negatively charged species (such as a F-ligand of an anion) making an approach to the triangular faces containing the two non-bonding electron pairs, as illustrated in Figure 4. It is significant that the F(1)-Xe-F(2) angle of Figure 3 is 154° and not 180°, and that all four F atoms close to the Xe atom are in the same plane.

It is instructive to compare XeF_3^+ with XeF^+ and XeF_5^+. In XeF^+ we have three non-bonding valence-electron pairs, therefore, the xenon coordination is pseudo tetrahedral as illustrated in Figure 4. This model indicates that a negatively charged species approaching XeF^+ would 'see' the greatest positive charge when placed on axis <u>trans</u> to the F-ligand. This model accounts for the geometry of the $XeF^+Sb_2F_{11}^-$ arrangement reported by Peacock and his coworkers and for the structure of $XeF^+RuF_6^-$ recently determined in these laboratories[12a]. On the other hand, the XeF_5^+ ion possesses only one non-bonding xenon valence-electron pair and the xenon coordination is pseudo octahedral. The crystal structures of the XeF_5^+ salts[12,13,14,15] are in excellent accord with the maximum polarizing capability of this ion being directed in a cone about the symmetry axis as shown in Figure 4.

We, therefore, believe that the XeF_3 species seen in the $XeF_3^+Sb_2F_{11}^-$ structure represents the geometry of the cation XeF_3^+. We anticipate that the close similarity in shape observed for other isoelectronic species, e.g. SF_3^+ and PF_3 (ref. 2), and XeF_5^+ and IF_5 (ref 12a), will hold for XeF_3^+ and IF_3 and that the F(equatorial)-I-F(axial) angle will again be close to 80°.

As may be seen from Table IV and Figure 2 the axial bonds in XeF_3^+, ClF_3 and BrF_3 are significantly longer than the equatorial. All bonds are shorter than in XeF_4, where Xe-F = 1.95 Å[16]. Evidently the equatorial F-ligand is more strongly bound than the axial ligands. This is in accord with the Pimentel and Rundle models[17], in which the axial bonds are formulated as three center bonds (with the bonds amounting to single electron bonds) and the equatorial bond represented as an electron-pair bond. Alternatively the greater length of the axial bonds can be attributed, on the basis of the electron pair repulsion model,[9] to the greater repulsive interaction of the axial-F ligands with the non-bonding electron pairs (which are at 90°); the equatorial ligand is at 120° from those electron pairs.

The length of the equatorial Xe-F^+ bond compares closely with that of Xe-F^+, as predicted[18] on the basis of the Xe-F bonds in XeF_2 being of bond order 0.5, and with that observed[6] in $XeF^+Sb_2F_{11}^-$. This is certainly consistent with an electron-pair representation. The axial Xe-F bonds are significantly shorter than Xe-F in XeF_4, but this shortening can be attributed to increase in the Xe-F bond polarity following the loss of F^- and consequent increase in the effective positive charge of the xenon atom.

ACKNOWLEDGMENT

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5. Table II will appear 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 St., N.W., Washington, D.C. 20036, by referring to code number INORG-00-0000. Remit check or money order for $0.00 for photocopy or $0.00 for microfiche.
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TABLE I

Positional and Thermal Parameters for $XeF_3^+Sb_2F_{11}^-$
(Standard Deviations are in Parentheses)

Atom	x	y	z	B11	B22	B33	B12	B13	B23
Xe	.29614(8)	.74522(6)	.18648(6)	3.01(2)	2.69(2)	2.17(2)	1.54(2)	1.19(2)	.12(1)
Sb(1)	.12219(8)	.28979(6)	.50926(6)	2.37(2)	2.56(2)	1.83(2)	1.16(2)	.87(2)	- .37(1)
Sb(2)	.35701(8)	.22795(6)	.20527(7)	2.75(2)	2.71(2)	1.91(2)	1.16(2)	1.09(2)	- .42(1)
F(1)	.1925(7)	.2154(6)	.3502(7)	3.2(2)	3.2(2)	3.2(2)	1.0(2)	1.8(2)	- .6(2)
F(2)	.1869(9)	.4790(6)	.3518(7)	4.7(3)	3.6(2)	3.2(2)	2.4(2)	1.8(2)	.4(2)
F(3)	.3785(8)	.3544(7)	.6376(8)	3.2(2)	4.3(3)	3.8(2)	1.6(2)	- .6(2)	-1.7(2)
F(4)	.318(1)	.0264(6)	.3119(8)	5.7(3)	3.1(2)	4.3(3)	2.5(2)	2.6(2)	.7(2)
F(5)	.078(1)	.0993(6)	.6485(8)	6.1(3)	3.1(2)	3.6(2)	1.9(2)	3.1(2)	.8(2)
F(6)	.134(1)	.1604(8)	.0228(8)	5.3(3)	6.1(3)	2.9(2)	2.3(3)	.2(2)	-2.1(2)
F(7)	.510(1)	.2383(8)	.0782(8)	5.0(3)	5.9(3)	4.1(2)	2.6(3)	3.1(2)	- .3(2)
F(8)	.057(1)	.3681(8)	.6462(8)	7.1(4)	5.8(3)	4.1(2)	3.9(3)	3.2(3)	- .3(2)
F(9)	.273(1)	.8988(7)	-.0048(7)	5.5(3)	3.6(2)	2.5(2)	1.8(2)	1.3(2)	1.0(2)
F(10)	.0531(9)	.6367(7)	.0420(8)	3.4(2)	4.6(3)	3.4(2)	1.8(2)	- .4(2)	-1.2(2)
F(11)	.5350(8)	.9022(6)	.2669(8)	3.5(2)	3.3(2)	4.6(3)	1.4(2)	1.3(2)	- .2(2)
F(12)	-.1162(9)	.2269(9)	.3476(9)	2.8(2)	6.6(4)	4.2(3)	1.3(2)	.1(2)	-2.1(2)
F(13)	.5594(8)	.2897(7)	.4117(7)	3.4(2)	5.8(3)	2.7(2)	2.2(2)	.5(2)	-1.0(2)
F(14)	.3726(9)	.4274(5)	.1226(7)	4.7(3)	2.1(2)	3.9(2)	1.2(2)	2.2(2)	.4(2)

NOTE FOR PRINTER: Table II will appear only in the microfilm version of this paper.

Table II

Observed Structure Factors, Standard Deviations, and Differences (X1.0) for $XeF_3^+Sb_2F_{11}^-$

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X 1.0) FOR XEF3 SB2F11 F(0,0,0) = 560

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	-6	5	3	1*	H,K=		0,	6	1	39	0	2	-3	52	0	-0
1	39	0	4	-5	60	1	5	-7	35	1	1	2	22	0	1	-2	5	6	4*
2	44	0	1	-4	12	2	2	-6	14	1	1	3	11	2	0	-1	20	0	-0
3	103	1	5	-3	23	0	5	-5	36	1	-1	4	26	1	1	0	64	1	2
4	58	0	1	-2	106	1	-2	-4	42	0	-2	5	18	1	-0	1	0	6	-0*
5	56	0	-5	-1	94	1	-4	-3	40	0	3	6	3	5	-1*	2	5	2	1*
6	95	1	3	0	27	1	-0	-2	67	0	-1	7	6	3	5*	3	64	0	3
7	81	0	-3	1	44	0	-3	-1	17	1	1	H,K=		0,	10	4	21	2	1
8	14	0	3	2	11	3	-6*	0	89	1	-6	-3	4	5	3*	H,K=		1,	-8
9	10	1	-1	3	47	2	-3	1	76	1	-8	-2	46	0	4	-8	21	1	1
H,K=		0,	1	4	57	0	4	2	43	1	-2	-1	4	7	2*	-7	45	0	1
-9	2	6	2*	5	37	1	6	3	101	0	0	0	4	5	-0*	-6	2	4	0*
-8	17	1	2	6	56	2	5	4	28	1	3	1	62	0	4	-5	56	1	-1
-7	23	0	1	7	36	0	-0	5	55	0	2	2	19	1	1	-4	27	0	-2
-6	19	1	3	8	3	4	-2*	6	31	0	-1	3	17	0	2	-3	25	1	-1
-5	36	1	7	9	27	0	-3	7	6	2	5*	4	37	0	0	-2	69	0	0
-4	45	1	-2	H,K=		0,	4	8	51	0	-1	5	35	0	3	-1	11	1	3
-3	25	0	0	-8	7	1	-2	H,K=		0,	7	6	13	1	3	0	36	1	-1
-2	41	0	-2	-7	61	0	-1	-6	24	0	0	H,K=		0,	11	1	46	0	-1
-1	41	1	0	-6	27	1	-4	-5	56	1	4	-1	9	3	3*	2	43	1	2
0	7	4	-2*	-5	40	0	0	-4	7	2	2*	0	0	4	-3*	3	31	1	-1
1	29	0	-0	-4	51	0	0	-3	37	0	-1	1	26	1	4	4	29	1	2
2	34	0	1	-3	119	0	6	-2	60	1	1	2	10	1	1	5	32	1	0
3	40	1	7	-2	78	0	-1	-1	8	1	0	3	14	1	5	H,K=		1,	-7
4	5	2	1*	-1	81	1	-1	0	5	3	2*	4	8	2	-2*	-9	15	1	1
5	4	3	-4*	0	135	1	-12	1	63	1	-1	H,K=		1,	-12	-8	27	1	-0
6	36	1	4	1	59	1	-2	2	59	1	-2	-2	10	1	4	-7	37	1	-4
7	43	0	-1	2	55	1	-0	3	36	0	1	-1	6	4	2*	-6	24	0	-2
8	6	2	5*	3	140	1	5	4	36	1	-1	H,K=		1,	-11	-5	17	1	5
9	20	1	-1	4	10	1	6	5	34	0	0	-5	8	5	7*	-4	67	0	4
H,K=		0,	2	5	46	0	-0	6	17	1	2	-4	21	0	4	-3	57	0	-1
-9	15	1	-2	6	64	1	-4	7	8	1	0	-3	32	0	3	-2	8	2	-2*
-8	12	1	-8	7	32	1	-4	8	13	1	0	-2	1	6	-3*	-1	32	0	-1
-7	85	0	-4	8	52	0	-5	H,K=		0,	8	-1	19	1	1	0	78	0	-0
-6	43	1	4	9	0	6	-1*	-5	34	1	1	0	50	1	5	1	9	1	3
-5	50	0	1	H,K=		0,	5	-4	25	1	1	1	7	3	2*	2	8	1	3*
-4	72	1	1	-7	12	1	-0	-3	6	2	1*	2	8	1	3	3	57	0	-1
-3	174	3	0	-6	22	1	-1	-2	61	1	2	H,K=		1,	-10	4	22	0	-1
-2	29	0	-2	-5	45	0	3	-1	3	4	3*	-6	18	1	0	5	18	1	0
-1	47	1	-2	-4	2	5	-1*	0	41	1	0	-5	22	1	2	6	46	0	3
0	237	6	-36	-3	30	0	0	1	59	0	-3	-4	20	0	-0	H,K=		1,	-6
1	16	1	4	-2	99	0	1	2	29	1	-2	-3	37	1	3	-9	33	0	-3
2	29	0	-1	-1	81	0	1	3	32	0	1	-2	32	0	3	-8	31	1	-2
3	168	3	11	0	30	1	-1	4	46	0	4	-1	0	6	-2*	-7	31	0	3
4	65	0	-0	1	42	1	-2	5	49	0	1	0	40	1	0	-6	23	0	0
5	70	0	-7	2	42	1	-1	6	25	1	-1	1	17	1	2	-5	106	0	2
6	91	1	1	3	23	2	2	7	7	2	-3*	2	16	1	1	-4	60	0	-1
7	53	0	4	4	72	1	-1	H,K=		0,	9	3	25	1	3	-3	11	2	1
8	34	0	1	5	49	0	3	-4	8	2	-0*	H,K=		1,	-9	-2	120	1	-4
9	11	1	-4	6	44	1	0	-3	15	1	-0	-7	30	0	2	-1	33	0	-1
H,K=		0,	3	7	24	0	-2	-2	54	1	6	-6	21	0	2	0	58	0	-2
-8	25	1	2	8	10	3	-5*	-1	11	1	1	-5	12	1	-2	1	111	1	-4
-7	20	1	-3	9	24	0	4	0	6	1	2	-4	44	1	1	2	48	0	-4

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF3 S82F11

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	21	1	-1	5	40	0	2	4	105	1	6	2	52	0	1	6	60	0	3
4	57	0	3	6	29	0	2	5	46	0	-1	3	37	0	2	7	11	2	4
5	49	0	1	7	7	2	5*	6	31	1	3	4	108	0	-8	8	2	5	-3*
6	5	2	1*	8	39	0	-2	7	38	0	-4	5	64	0	0	H,K=		1,	7
7	16	1	-0	H,K=		1,	-2	8	38	0	1	6	18	1	1	-6	8	2	-1*
H,K=		1,	-5	-9	56	0	-4	9	17	1	-2	7	36	1	6	-5	26	0	1
-9	16	1	-0	-8	58	0	-7	H,K=		1,	1	8	28	0	3	-4	44	1	2
-8	24	0	4	-7	41	0	-2	-9	7	1	1*	9	2	5	-2*	-3	9	2	2*
-7	32	0	1	-6	110	0	3	-8	15	4	-2*	H,K=		1,	4	-2	15	0	-2
-6	34	0	-1	-5	122	1	13	-7	48	0	6	-8	3	8	3*	-1	38	0	2
-5	27	0	-1	-4	56	0	1	-6	22	0	4	-7	38	0	-0	0	2	8	1*
-4	46	0	2	-3	55	0	-3	-5	36	0	-2	-6	54	0	2	1	13	1	1
-3	62	0	-2	-2	271	0	2	-4	60	0	-5	-5	29	0	5	2	13	1	2
-2	12	1	-1	-1	13	1	-2	-3	15	0	8	-4	81	1	1	3	33	0	-2
-1	53	0	1	0	9	2	0*	-2	72	0	3	-3	50	0	-2	4	14	1	-0
0	56	0	-3	1	216	0	-4	-1	62	0	-2	-2	69	0	-3	5	6	1	1*
1	37	0	-1	2	26	1	0	0	85	0	-6	-1	125	0	-3	6	2	4	-3*
2	14	0	-3	3	57	0	1	1	128	0	5	0	26	0	-2	7	13	2	1
3	68	1	3	4	114	1	3	2	18	0	1	1	112	0	-3	H,K=		1,	8
4	12	1	0	5	92	1	-6	3	43	0	-1	2	76	0	-2	-5	17	1	1
5	31	0	1	6	20	0	-3	4	98	0	11	3	93	0	3	-4	64	0	5
6	36	0	0	7	29	1	3	5	68	1	2	4	58	1	0	-3	6	2	-0*
7	8	1	-4	8	44	0	-1	6	5	2	4*	5	29	0	1	-2	5	3	4*
H,K=		1,	-4	H,K=		1,	-1	7	45	0	-5	6	67	0	-0	-1	65	1	3
-9	49	1	-3	-9	10	2	6	8	44	0	3	7	8	1	0	0	12	1	-2
-8	40	0	-5	-8	5	2	-3*	9	0	4	-4*	8	17	1	-4	1	24	0	2
-7	46	1	-2	-7	21	0	3	H,K=		1,	2	H,K=		1,	5	2	77	0	1
-6	74	0	1	-6	13	1	6	-9	53	1	-5	-7	43	0	3	3	47	0	1
-5	159	1	6	-5	7	2	1*	-8	12	1	6	-6	9	3	-0*	4	14	0	3
-4	26	0	-0	-4	14	0	1	-7	38	0	-2	-5	39	0	-1	5	30	0	0
-3	31	0	-2	-3	4	5	2*	-6	89	0	4	-4	46	0	1	6	51	0	3
-2	99	0	-2	-2	62	0	4	-5	80	0	0	-3	28	0	2	7	12	2	-4*
-1	16	0	1	-1	37	0	1	-4	86	1	1	-2	38	0	-3	H,K=		1,	9
0	60	0	-2	0	35	0	2	-3	65	0	0	-1	62	0	-1	-4	27	1	3
1	220	0	-12	1	123	0	9	-2	138	0	0	0	41	0	-1	-3	12	2	3*
2	84	0	-5	2	41	0	0	-1	56	0	-1	1	31	0	-1	-2	0	5	-2*
3	20	0	1	3	10	1	0	0	26	1	-3	2	27	0	-1	-1	20	0	4
4	78	1	4	4	53	0	10	1	132	0	-2	3	43	1	3	0	0	4	-2*
5	67	0	3	5	66	0	-4	2	58	0	3	4	41	0	1	1	9	1	1
6	21	1	-7	6	9	3	1*	3	107	0	3	5	33	1	1	2	9	1	3
7	30	1	-5	7	36	0	2	4	119	1	5	6	11	1	-5	3	5	2	3*
8	44	0	-2	8	46	0	4	5	18	0	-3	7	29	1	4	4	7	3	2*
H,K=		1,	-3	9	9	2	-2*	6	64	0	-1	8	17	1	-2	5	5	6	2*
-9	17	1	-1	H,K=		1,	0	7	18	0	-7	H,K=		1,	6	6	5	2	0*
-8	15	1	2	-9	59	0	-5	8	25	1	4	-7	31	1	1	H,K=		1,	10
-7	7	6	2*	-8	33	0	8	9	30	0	-4	-6	33	0	-0	-2	0	5	-6*
-6	6	1	4*	-7	30	1	-1	H,K=		1,	3	-5	8	2	-3*	-1	59	0	8
-5	43	1	1	-6	117	0	2	-8	32	0	-1	-4	77	0	0	0	6	2	0*
-4	24	0	-5	-5	110	1	-1	-7	45	0	3	-3	15	1	1	1	8	4	2*
-3	45	0	3	-4	65	0	5	-6	1	4	-5*	-2	33	0	0	2	54	0	4
-2	44	0	-2	-3	34	0	0	-5	10	1	-1	-1	83	0	-2	3	25	0	5
-1	24	1	1	-2	262	0	9	-4	88	0	1	0	29	0	-1	4	17	2	2
0	44	1	-2	-1	69	0	1	-3	72	0	0	1	62	0	-1	H,K=		2,	-12
1	65	0	-2	0	19	1	-0	-2	97	0	1	2	100	1	-1	-4	24	1	3
2	39	0	2	1	261	0	8	-1	53	0	-3	3	78	0	-0	-3	0	5	-3*
3	52	0	-4	2	14	1	-0	0	31	0	-1	4	29	0	-3	-2	21	1	3
4	59	0	2	3	104	0	1	1	30	0	3	5	33	0	1	-1	18	1	3

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF3 SBZF11

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
0	8	1	3	-6	47	0	-1	-4	167	1	3	-6	27	1	6	-6	87	0	2
H,K=		2,	-11	-5	11	1	-0	-3	20	1	2	-5	55	0	3	-5	48	0	3
-6	38	0	-0	-4	25	0	1	-2	48	0	-1	-4	82	0	-2	-4	41	1	1
-5	32	0	1	-3	47	0	0	-1	149	0	-9	-3	56	0	2	-3	159	0	2
-4	11	1	2	-2	53	0	-3	0	3	4	-1*	-2	83	0	7	-2	13	0	-2
-3	27	1	3	-1	31	0	-1	1	48	0	2	-1	169	0	1	-1	45	0	-2
-2	48	0	3	0	5	2	3*	2	143	1	3	0	45	0	2	0	70	0	-2
-1	7	2	3*	1	61	0	1	3	78	0	10	1	46	0	4	1	93	0	3
0	15	1	2	2	28	1	2	4	30	0	-3	2	5	0	-81	2	111	1	5
1	62	0	6	3	27	0	-2	5	38	0	1	3	59	0	2	3	73	0	-1
2	4	6	-0*	4	48	0	3	6	36	0	-6	4	16	0	-1	4	103	1	-0
H,K=		2,	-10	5	10	1	2	7	16	1	-4	5	74	1	-9	5	21	0	-1
-7	32	0	-1	6	37	0	2	H,K=		2,	-3	6	58	0	-4	6	2	4	-2*
-6	9	1	-2	H,K=		2,	-6	-10	9	1	2	7	11	1	5	7	58	1	-4
-5	7	1	1	-9	16	1	-2	-9	9	3	-1*	8	21	1	3	8	10	2	1*
-4	49	0	3	-8	49	0	-4	-8	13	1	3	H,K=		2,	0	H,K=		2,	3
-3	10	1	1	-7	82	0	-3	-7	0	7	-2*	-9	21	0	-0	-8	14	2	-0
-2	13	1	3	-6	42	1	1	-6	18	0	-7	-8	70	1	-7	-7	32	0	0
-1	40	0	0	-5	34	1	3	-5	68	0	2	-7	37	0	1	-6	36	0	3
0	28	1	1	-4	122	1	2	-4	79	0	1	-6	84	0	0	-5	31	0	-2
1	14	1	-2	-3	4	6	1*	-3	69	0	3	-5	58	0	6	-4	23	1	3
2	31	0	1	-2	10	2	-4	-2	13	0	-1	-4	101	0	6	-3	41	1	1
3	23	0	1	-1	165	1	-8	-1	134	0	-8	-3	128	0	3	-2	62	0	1
H,K=		2,	-9	0	66	0	-2	0	15	1	-2	-2	0	6	-0*	-1	81	0	-4
-8	10	1	-2	1	20	0	0	1	52	0	1	-1	159	0	-13	0	49	0	-3
-7	10	1	2	2	78	0	2	2	105	1	6	0	66	0	-0	1	3	2	2*
-6	48	1	-2	3	33	0	1	3	73	0	2	1	92	0	3	2	82	0	-2
-5	24	1	1	4	10	1	-4	4	21	1	-1	2	125	0	8	3	19	0	-1
-4	14	1	4	5	45	0	0	5	64	1	7	3	3	2	-4*	4	7	1	3
-3	32	1	-0	6	39	0	1	6	57	0	-3	4	90	1	4	5	40	0	4
-2	68	0	-0	7	6	2	1*	7	14	1	-2	5	46	0	-1	6	18	1	1
-1	15	0	2	H,K=		2,	-5	8	14	1	-5	6	11	1	-7	7	18	1	-4
0	14	0	3	-10	12	1	1	H,K=		2,	-2	7	43	1	-1	8	20	1	1
1	66	1	0	-9	10	1	-1	-10	15	1	0	8	11	1	-1	H,K=		2,	4
2	8	1	4	-8	5	2	3*	-9	20	0	1	H,K=		2,	1	-8	24	0	-1
3	23	1	1	-7	6	5	2*	-8	71	0	-7	-9	21	1	0	-7	21	0	-0
4	47	1	3	-6	28	0	-0	-7	62	0	2	-8	16	1	3	-6	74	0	0
H,K=		2,	-8	-5	7	1	7	-6	73	0	2	-7	24	1	2	-5	39	0	-0
-9	18	1	1	-4	44	0	1	-5	90	0	4	-6	65	0	2	-4	12	2	1
-8	28	1	-1	-3	16	0	2	-4	167	0	11	-5	56	0	-0	-3	134	1	1
-7	57	0	-1	-2	10	0	0	-3	104	0	3	-4	102	0	6	-2	7	1	4
-6	34	1	-2	-1	82	0	-4	-2	20	2	1	-3	40	0	1	-1	31	0	0
-5	6	1	1*	0	8	1	5	-1	225	0	-6	-2	49	0	0	0	132	1	-6
-4	95	0	1	1	69	0	1	0	30	1	0	-1	71	0	-3	1	87	1	-1
-3	0	4	-2*	2	97	1	-2	1	37	0	-1	0	56	0	-4	2	67	1	-3
-2	16	1	0	3	36	0	6	2	113	1	3	1	54	0	1	3	65	0	-3
-1	89	0	-2	4	39	0	3	3	52	0	6	2	197	1	13	4	68	1	0
0	34	0	3	5	21	0	6	4	62	1	1	3	31	0	-0	5	4	5	2*
1	23	0	1	6	52	1	-5	5	47	0	5	4	6	6	-2*	6	16	1	5
2	49	0	-1	7	12	1	-0	6	23	1	-8	5	51	0	-2	7	62	1	-1
3	43	1	-3	H,K=		2,	-4	7	25	2	-3	6	38	1	5	8	7	1	6
4	6	1	5*	-10	24	0	-5	8	5	3	3*	7	14	1	2	H,K=		2,	5
5	26	0	3	-9	20	1	-3	H,K=		2,	-1	8	26	1	5	-7	25	1	-0
H,K=		2,	-7	-8	67	1	-4	-10	14	2	-0	H,K=		2,	2	-6	17	1	3
-9	26	1	-2	-7	75	0	5	-9	16	1	1	-9	27	2	-2	-5	12	1	1
-8	10	4	0*	-6	63	0	-1	-8	25	0	-1	-8	53	1	-3	-4	14	2	-1
-7	5	4	4*	-5	73	0	1	-7	36	0	-0	-7	3	4	-0*	-3	28	0	-2

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF3 S82F11

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	6	1	4	0	7	2	-2*	-8	8	4	5*	-3	145	0	3	-3	176	0	11
-1	33	0	0	1	16	0	2	-7	41	0	-2	-2	1	4	0*	-2	165	0	7
0	11	1	4	2	13	1	3	-6	82	0	1	-1	18	1	1	-1	30	0	-3
1	34	0	1	3	10	1	-1	-5	30	0	-1	0	123	1	-16	0	49	0	0
2	23	0	-1	4	11	3	-2*	-4	9	1	3	1	44	0	-0	1	23	0	4
3	10	1	5	H,K=	2,	10		-3	104	0	-6	2	36	1	6	2	104	0	7
4	13	1	3	-1	4	8	3*	-2	40	0	1	3	102	1	12	3	41	0	-4
5	18	1	6	0	45	1	6	-1	20	0	-5	4	71	0	4	4	27	0	-2
6	8	1	4	1	6	2	2*	0	66	0	-2	5	17	1	-5	5	49	0	6
7	17	1	-2	2	21	1	3	1	16	1	-5	6	24	2	1	6	4	3	-6*
H,K=	2,	6		H,K=	3,-12			2	6	3	-1*	7	44	0	-2	7	7	8	-4*
-7	25	0	-1	-5	7	1	6*	3	36	0	-1	H,K=	3,	-4		H,K=	3,	-1	
-6	62	0	2	-4	11	2	2	4	32	1	2	-10	52	0	-3	-10	23	1	-3
-5	22	0	-1	-3	27	1	1	5	13	3	-0*	-9	29	1	-1	-9	21	0	0
-4	17	1	3	-2	12	1	0	H,K=	3,	-7		-8	43	0	0	-8	23	1	1
-3	85	0	-0	-1	5	2	1*	-9	13	1	-3	-7	72	1	-4	-7	49	0	1
-2	15	1	2	0	30	0	2	-8	17	1	1	-6	90	0	6	-6	101	1	-1
-1	22	0	3	H,K=	3,-11			-7	12	1	1	-5	51	0	0	-5	29	0	3
0	105	1	-1	-7	16	1	0	-6	38	0	1	-4	36	0	2	-4	97	1	4
1	48	0	-4	-6	9	1	1	-5	59	0	-1	-3	146	0	8	-3	78	0	9
2	24	0	2	-5	36	1	-2	-4	7	2	2*	-2	71	0	-0	-2	33	0	2
3	61	0	2	-4	34	0	0	-3	75	0	-3	-1	8	1	-4	-1	28	0	-5
4	60	0	5	-3	30	0	1	-2	12	1	1	0	85	0	-4	0	154	0	13
5	24	0	-4	-2	20	2	3	-1	18	1	0	1	8	1	1	1	45	0	0
6	21	1	1	-1	52	0	3	0	92	0	-4	2	68	0	3	2	8	1	0
7	47	0	2	0	19	1	3	1	26	0	0	3	43	0	-2	3	124	1	12
H,K=	2,	7		1	14	1	2	2	45	0	4	4	32	0	-7	4	44	0	0
-6	17	2	2	2	41	1	1	3	44	1	5.	5	32	1	-3	5	34	1	1
-5	14	1	2	H,K=	3,-10			4	59	1	1	6	11	3	-4*	6	37	0	-2
-4	8	1	6	-8	6	2	-2*	5	23	0	-1	7	5	8	4*	7	41	0	-0
-3	14	0	4	-7	19	1	-3	6	15	1	2	H,K=	3,	-3		8	13	1	-1
-2	12	3	1*	-6	57	0	-1	H,K=	3,	-6	-10	31	1	-5		H,K=	3,	0	
-1	9	2	5	-5	0	4	-3*	-10	50	0	-4	-9	31	0	-2	-9	16	1	-3
0	6	3	1*	-4	7	1	1	-9	41	0	-0	-8	11	1	5	-8	54	0	-1
1	5	3	2*	-3	51	0	-2	-8	17	1	-2	-7	51	0	-1	-7	39	0	1
2	5	3	3*	-2	12	2	2	-7	52	1	-3	-6	41	0	-1	-6	13	1	2
3	16	2	-3	-1	5	2	-2*	-6	97	0	1	-5	13	0	6	-5	154	1	2
4	14	2	1	0	51	1	1	-5	27	0	1	-4	115	0	4	-4	6	1	4
5	6	2	-2*	1	39	1	1	-4	31	0	1	-3	212	0	11	-3	81	0	-0
6	11	2	-1	2	7	2	3*	-3	131	1	0	-2	21	0	2	-2	84	0	-3
H,K=	2,	8		3	26	1	0	-2	17	1	-0	-1	24	0	1	-1	28	0	-7
-5	17	1	0	H,K=	3,	-9		-1	21	0	1	0	67	0	3	0	51	0	1
-4	20	1	2	-8	31	0	-2	0	98	1	-6	1	62	0	1	1	145	1	10
-3	69	1	6	-7	0	7	-1*	1	6	1	0	2	10	2	-2	2	160	1	10
-2	0	4	-0*	-6	24	0	-1	2	8	1	-0	3	155	1	13	3	31	0	-4
-1	3	4	3*	-5	48	0	-1	3	43	0	-2	4	75	0	-6	4	29	0	-6
0	67	1	5	-4	29	0	2	4	34	0	4	5	24	0	3	5	60	0	5
1	14	3	0*	-3	43	0	-2	5	13	1	-2	6	35	0	-0	6	9	1	6
2	21	1	3	-2	4	7	0*	6	20	1	-3	7	44	0	4	7	6	4	4*
3	44	0	1	-1	46	0	-0	H,K=	3,	-5		H,K=	3,	-2		8	36	0	-4
4	41	1	4	0	41	1	3	-10	21	1	-2	-10	43	1	-5	H,K=	3,	1	
5	19	1	-1	1	24	0	-3	-9	21	0	-0	-9	8	1	4	-9	20	0	-0
6	17	2	1	2	48	0	0	-8	8	2	-1*	-8	51	1	-1	-8	27	0	1
H,K=	2,	9		3	26	0	1	-7	38	0	-1	-7	65	0	-2	-7	31	0	0
-3	3	6	3*	4	35	1	2	-6	47	0	2	-6	58	0	5	-6	49	0	3
-2	16	1	2	H,K=	3,	-8	-5	7	1	-4	-5	114	0	4	-5	20	1	3	
-1	18	1	2	-9	42	0	-3	-4	44	0	0	-4	11	1	3	-4	79	0	-2

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF3 S82F11

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	6	1	4	0	7	2	-2*	-8	8	4	5*	-3	145	0	3	-3	176	0	11
-1	33	0	0	1	16	0	2	-7	41	0	-2	-2	1	4	0*	-2	165	0	7
0	11	1	4	2	13	1	3	-6	82	0	1	-1	18	1	1	-1	30	0	-3
1	34	0	1	3	10	1	-1	-5	30	0	-1	0	123	1	-16	0	49	0	0
2	23	0	-1	4	11	3	-2*	-4	9	1	3	1	44	0	-0	1	23	0	4
3	10	1	5	H,K=		2,	10	-3	104	0	-6	2	36	1	6	2	104	0	7
4	13	1	3	-1	4	8	3*	-2	40	0	1	3	102	1	12	3	41	0	-4
5	18	1	6	0	45	1	6	-1	20	0	-5	4	71	0	4	4	27	0	-2
6	8	1	4	1	6	2	2*	0	66	0	-2	5	17	1	-5	5	49	0	6
7	17	1	-2	2	21	1	3	1	16	1	-5	6	24	2	1	6	4	3	-6*
H,K=		2,	6	H,K=		3,	-12	2	6	3	-1*	7	44	0	-2	7	7	8	-4*
-7	25	0	-1	-5	7	1	6*	3	36	0	-1	H,K=		3,	-4	H,K=		3,	-1
-6	62	0	2	-4	11	2	2	4	32	1	2	-10	52	0	-3	-10	23	1	-3
-5	22	0	-1	-3	27	1	1	5	13	3	-0*	-9	29	1	-1	-9	21	0	0
-4	17	1	3	-2	12	1	0	H,K=		3,	-7	-8	43	0	0	-8	23	1	1
-3	85	0	-0	-1	5	2	1*	-9	13	1	-3	-7	72	1	-4	-7	49	0	1
-2	15	1	2	0	30	0	2	-8	17	1	1	-6	90	0	6	-6	101	1	-1
-1	22	0	3	H,K=		3,	-11	-7	12	1	1	-5	51	0	0	-5	29	0	3
0	105	1	-1	-7	16	1	0	-6	38	0	1	-4	36	0	2	-4	97	1	4
1	48	0	-4	-6	9	1	1	-5	59	0	-1	-3	146	0	8	-3	78	0	9
2	24	0	2	-5	36	1	-2	-4	7	2	2*	-2	71	0	-0	-2	33	0	2
3	61	0	2	-4	34	0	0	-3	75	0	-3	-1	8	1	-4	-1	28	0	-5
4	60	0	5	-3	30	0	1	-2	12	1	1	0	85	0	-4	0	154	0	13
5	24	0	-4	-2	20	2	3	-1	18	1	0	1	8	1	1	1	45	0	0
6	21	1	1	-1	52	0	3	0	92	0	-4	2	68	0	3	2	8	1	0
7	47	0	2	0	19	1	3	1	26	0	0	3	43	0	-2	3	124	1	12
H,K=		2,	7	1	14	1	2	2	45	0	4	4	32	0	-7	4	44	0	0
-6	17	2	2	2	41	1	1	3	44	1	5	5	32	1	-3	5	34	1	1
-5	14	1	2	H,K=		3,	-10	4	59	1	1	6	11	3	-4*	6	37	0	-2
-4	8	1	6	-8	6	2	-2*	5	23	0	-1	7	5	8	4*	7	41	0	-0
-3	14	0	4	-7	19	1	-3	6	15	1	2	H,K=		3,	-3	8	13	1	-1
-2	12	3	1*	-6	57	0	-1	H,K=		3,	-6	-10	31	1	-5	H,K=		3,	0
-1	9	2	5	-5	0	4	-3*	-10	50	0	-4	-9	31	0	-2	-9	16	1	-3
0	6	3	1*	-4	7	1	1	-9	41	0	-0	-8	11	1	5	-8	54	0	-1
1	5	3	2*	-3	51	0	-2	-8	17	1	-2	-7	51	0	-1	-7	39	0	1
2	5	3	3*	-2	12	2	2	-7	52	1	-3	-6	41	0	-1	-6	13	1	2
3	16	2	-3	-1	5	2	-2*	-6	97	0	1	-5	13	0	6	-5	154	1	2
4	14	2	1	0	51	1	1	-5	27	0	1	-4	115	0	4	-4	6	1	4
5	6	2	-2*	1	39	1	1	-4	31	0	1	-3	212	0	11	-3	81	0	-0
6	11	2	-1	2	7	2	3*	-3	131	1	0	-2	21	0	2	-2	84	0	-3
H,K=		2,	8	3	26	1	0	-2	17	1	-0	-1	24	0	1	-1	28	0	-7
-5	17	1	0	H,K=		3,	-9	-1	21	0	1	0	67	0	3	0	51	0	1
-4	20	1	2	-8	31	0	-2	0	98	1	-6	1	62	0	1	1	145	1	10
-3	69	1	6	-7	0	7	-1*	1	6	1	0	2	10	2	-2	2	160	1	10
-2	0	4	-0*	-6	24	0	-1	2	8	1	-0	3	155	1	13	3	31	0	-4
-1	3	4	3*	-5	48	0	-1	3	43	0	-2	4	75	0	-6	4	29	0	-6
0	67	1	5	-4	29	0	2	4	34	0	4	5	24	0	3	5	60	0	5
1	14	3	0*	-3	43	0	-2	5	13	1	-2	6	35	0	-0	6	9	1	6
2	21	1	3	-2	4	7	0*	6	20	1	-3	7	44	0	4	7	6	4	4*
3	44	0	1	-1	46	0	-0	H,K=		3,	-5	H,K=		3,	-2	8	36	0	-4
4	41	1	4	0	41	1	3	-10	21	1	-2	-10	43	1	-5	H,K=		3,	1
5	19	1	-1	1	24	0	-3	-9	21	0	-0	-9	8	1	4	-9	20	0	-0
6	17	2	1	2	48	0	0	-8	8	2	-1*	-8	51	1	-1	-8	27	0	1
H,K=		2,	9	3	26	0	1	-7	38	0	-1	-7	65	0	-2	-7	31	0	0
-3	3	6	3*	4	35	1	2	-6	47	0	2	-6	58	0	5	-6	49	0	3
-2	16	1	2	H,K=		3,	-8	-5	7	1	-4	-5	114	0	4	-5	20	1	3
-1	18	1	2	-9	42	0	-3	-4	44	0	0	-4	11	1	3	-4	79	0	-2

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF3 S82F11

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
0	90	0	1	2	44	0	-6	-6	15	1	2	0	28	0	-3	0	34	0	2
1	5	4	-9*	3	48	0	2	-5	16	1	3	1	18	1	-1	1	23	0	4
2	71	0	4	4	29	0	7	-4	35	1	0	2	38	0	2	2	61	1	5
3	59	1	10	5	5	3	3*	-3	15	1	0	H,K=	5,-10			3	41	0	-5
4	6	2	-5*	6	51	1	1	-2	15	1	-2	-8	24	1	-1	4	30	0	-4
5	19	1	-3	7	2	4	-6*	-1	61	0	-2	-7	38	1	-0	5	23	0	1
6	41	0	-4	H,K=	4,	2		0	19	1	2	-6	0	7	-1*	H,K=	5,	-6	
7	19	1	3	-9	23	1	0	1	6	5	1*	-5	11	1	-1	-10	3	4	-1*
H,K=	4,	-1		-8	39	1	-2	2	36	1	1	-4	27	2	1	-9	47	1	-2
-10	15	3	-1*	-7	73	1	1	3	38	1	3	-3	3	4	2*	-8	12	1	-1
-9	33	1	-0	-6	23	0	0	4	9	1	-4	-2	0	4	-1*	-7	1	5	-2*
-8	27	1	1	-5	15	2	-0	5	27	1	-2	-1	17	1	1	-6	66	0	2
-7	12	1	-0	-4	138	1	2	H,K=	4,	6	0	0	4	-5*	-5	10	1	2	
-6	39	0	2	-3	11	1	-0	-6	28	0	3	1	6	3	1*	-4	26	0	3
-5	73	0	2	-2	12	1	-2	-5	11	3	2*	2	5	2	1*	-3	49	0	2
-4	43	1	4	-1	119	1	-10	-4	44	0	3	3	5	3	2*	-2	43	0	-6
-3	75	0	3	0	61	0	1	-3	23	0	2	H,K=	5,	-9	-1	8	1	-4	
-2	86	1	-2	1	19	1	-2	-2	17	0	1	-9	13	3	-3*	0	54	0	0
-1	46	0	-2	2	50	0	4	-1	51	1	-0	-8	45	0	-3	1	61	0	-2
0	14	0	2	3	50	0	-2	0	3	4	-0*	-7	61	0	-2	2	20	1	4
1	128	1	10	4	9	1	-1	1	31	0	3	-6	16	0	3	3	25	1	1
2	6	1	1	5	12	1	1	2	28	1	5	-5	23	1	-0	4	18	1	-1
3	57	0	2	6	41	0	-1	3	17	1	3	-4	96	0	-2	5	10	11	7*
4	40	0	2	7	4	4	1*	4	33	1	1	-3	0	4	-3*	H,K=	5,	-5	
5	15	2	6	H,K=	4,	3		5	0	7	-4*	-2	12	1	2	-10	15	1	-0
6	42	0	3	-8	2	6	-4*	H,K=	4,	7	-1	86	0	-3	-9	0	5	-1*	
7	9	2	8*	-7	29	0	0	-4	28	1	1	0	26	0	-2	-8	71	1	-4
H,K=	4,	0		-6	7	1	5	-3	17	1	3	1	22	0	-2	-7	59	0	4
-9	38	1	-1	-5	1	4	0*	-2	22	0	1	2	57	1	3	-6	30	0	-2
-8	23	0	1	-4	30	1	-2	-1	31	1	-0	3	47	0	-0	-5	31	0	5
-7	97	0	2	-3	4	4	-1*	0	22	1	4	4	18	1	1	-4	142	1	8
-6	7	2	1*	-2	5	2	-2*	1	2	4	-0*	H,K=	5,	-8	-3	42	1	4	
-5	35	0	1	-1	79	0	-5	2	26	1	-0	-9	26	1	-1	-2	3	3	0*
-4	141	1	4	0	29	0	-1	3	22	1	0	-8	20	0	-1	-1	105	1	-8
-3	26	1	0	1	15	0	-0	4	1	7	-1*	-7	30	0	4	0	4	4	-3*
-2	46	0	-4	2	26	1	5	H,K=	4,	8	-6	28	0	-1	1	53	1	-3	
-1	127	1	-10	3	43	0	4	-2	18	1	2	-5	7	3	1*	2	86	1	1
0	97	1	-3	4	19	1	7	-1	29	1	3	-4	40	1	1	3	21	1	-2
1	5	1	3*	5	27	1	0	0	11	1	-1	-3	20	0	-0	4	39	0	2
2	80	0	1	6	50	1	-6	1	26	1	4	-2	16	2	-6	5	23	0	-2
3	73	1	2	H,K=	4,	4		2	14	1	3	-1	5	2	1*	6	28	0	5
4	10	2	-10	-7	53	0	1	H,K=	5,-12		0	27	1	4	H,K=	5,	-4		
5	10	1	0	-6	18	1	-1	-6	13	1	-0	1	11	1	4	-10	23	0	-3
6	44	0	-0	-5	10	1	1	-5	20	1	-1	2	6	1	-1*	-9	74	0	-4
7	17	1	1	-4	82	0	2	-4	26	0	-0	3	17	1	-2	-8	17	1	1
H,K=	4,	1		-3	12	1	1	-3	15	1	0	4	9	2	-1	-7	2	5	-5*
-9	14	1	-1	-2	20	1	-3	-2	7	1	3	H,K=	5,	-7	-6	97	0	6	
-8	3	5	-0*	-1	92	0	-4	-1	19	1	1	-10	21	1	1	-5	14	1	3
-7	7	2	-2*	0	28	1	-3	0	6	2	0*	-9	8	1	-0	-4	16	1	5
-6	24	0	-4	1	24	0	-0	H,K=	5,-11		-8	65	1	-5	-3	111	0	4	
-5	16	1	1	2	40	0	1	-7	47	0	1	-7	79	1	-2	-2	77	0	0
-4	60	0	-1	3	28	0	6	-6	10	3	5*	-6	10	1	2	-1	21	0	12
-3	15	1	2	4	25	1	1	-5	0	4	-7*	-5	37	0	5	0	67	1	5
-2	55	0	-1	5	12	1	1	-4	69	0	-2	-4	115	0	5	1	64	1	-1
-1	36	0	-2	6	25	1	3	-3	0	5	-2*	-3	45	0	1	2	19	0	-8
0	42	0	-2	H,K=	4,	5	-2	24	1	-1	-2	9	2	5	3	41	1	1	
1	63	0	-7	-7	20	1	2	-1	59	0	0	-1	129	1	-14	4	34	1	-1

OBSERVED STRUCTURES FACTORS (CONT) FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	23	0	7	-8	25	0	-1	0	67	0	0	-6	69	0	-3	-2	23	0	-4
6	16	1	6	-7	30	0	-2	1	43	0	3	-5	9	3	-3*	-1	38	0	-0
H,K=		5,	-3	-6	98	0	-0	2	13	1	-3	-4	2	4	-4*	0	79	1	2
-10	8	3	4*	-5	8	1	-0	3	41	1	2	-3	70	0	0	1	6	1	-2*
-9	9	6	-5*	-4	20	1	-2	4	51	0	0	-2	4	3	-1*	2	42	0	-2
-8	45	1	1	-3	95	0	1	5	6	4	1*	-1	20	0	-3	3	27	1	0
-7	40	0	2	-2	30	0	0	H,K=		5,	4	0	55	0	0	4	17	2	3
-6	41	0	4	-1	40	1	-3	-7	17	1	1	1	30	0	1	H,K=		6,	-6
-5	62	0	2	0	78	1	-1	-6	36	0	2	H,K=		6,	-10	-10	10	4	-2*
-4	87	1	1	1	54	0	-2	-5	25	0	0	-8	19	1	1	-9	11	1	-3
-3	84	0	7	2	5	1	1*	-4	10	1	-1	-7	3	4	0*	-8	70	0	-5
-2	13	0	0	3	23	1	-0	-3	50	0	1	-6	3	4	3*	-7	26	0	-4
-1	90	1	14	4	43	0	-5	-2	22	1	2	-5	21	2	-3	-6	30	1	-2
0	44	1	14	5	9	3	6*	-1	38	0	-2	-4	11	3	0*	-5	74	0	4
1	64	1	-2	6	8	3	-3*	0	31	1	3	-3	10	1	-0	-4	26	0	4
2	72	1	-2	H,K=		5,	1	1	0	6	-1*	-2	8	4	-1*	-3	16	1	1
3	5	7	-3*	-9	19	1	-3	2	37	1	2	-1	0	4	-1*	-2	50	0	-2
4	57	0	4	-8	14	1	-2	3	10	1	-4	0	15	1	3	-1	71	0	1
5	17	1	1	-7	15	1	-1	4	9	4	6*	1	19	2	-0	0	36	0	5
6	21	2	-9	-6	46	0	1	5	19	1	2	2	5	5	-0*	1	36	0	-3
H,K=		5,	-2	-5	0	5	-1*	H,K=		5,	5	H,K=		6,	-9	2	19	1	-8
-10	32	0	-3	-4	3	6	-2*	-6	33	1	2	-9	35	1	-1	3	17	1	1
-9	73	0	-3	-3	95	0	-4	-5	10	2	1*	-8	22	0	-1	4	28	1	4
-8	11	2	3	-2	36	0	-7	-4	14	1	2	-7	50	1	-6	H,K=		6,	-5
-7	29	0	-1	-1	27	1	-5	-3	45	1	-1	-6	77	1	-1	-10	41	1	-7
-6	102	1	4	0	74	1	-5	-2	7	1	4	-5	20	0	3	-9	6	2	4*
-5	17	1	3	1	47	0	-1	-1	0	4	-4*	-4	0	5	-3*	-8	46	0	-4
-4	19	0	2	2	14	0	3	0	48	0	0	-3	92	1	-3	-7	42	0	-2
-3	123	1	4	3	44	1	5	1	29	0	3	-2	5	8	4*	-6	56	1	5
-2	73	1	-7	4	70	0	1	2	10	1	3	-1	14	2	0	-5	74	0	3
-1	8	1	0	5	12	1	-7	3	34	0	-3	0	67	0	3	-4	5	5	2*
0	98	1	-1	6	8	2	-4*	4	26	0	1	1	27	1	-2	-3	73	0	2
1	61	1	1	H,K=		5,	2	H,K=		5,	6	2	34	0	-3	-2	45	0	5
2	6	1	5*	-8	26	1	-1	-5	36	0	3	3	28	0	-0	-1	52	0	-0
3	41	0	2	-7	27	0	-4	-4	13	1	2	H,K=		6,	-8	0	88	1	2
4	40	1	9	-6	76	1	1	-3	22	1	2	-9	8	1	2	1	36	0	-0
5	23	1	4	-5	23	0	-0	-2	29	0	2	-8	49	0	-2	2	62	1	-5
6	14	1	1	-4	6	1	-2*	-1	30	1	3	-7	23	0	-3	3	26	0	1
H,K=		5,	-1	-3	79	1	-0	0	20	2	2	-6	14	1	-4	4	5	7	-1*
-9	8	2	-4*	-2	8	1	1	1	10	2	-2	-5	41	1	-1	5	43	0	3
-8	26	0	-1	-1	34	0	-5	2	38	0	-1	-4	19	0	-0	H,K=		6,	-4
-7	14	0	2	0	44	0	-3	3	8	1	4	-3	6	4	3*	-10	7	7	2*
-6	63	0	5	1	17	0	0	H,K=		5,	7	-2	38	0	-3	-9	31	0	-3
-5	30	0	2	2	16	1	-0	-3	22	2	-1	-1	29	0	-3	-8	85	0	-3
-4	38	1	1	3	16	0	5	-2	6	6	1*	0	34	0	5	-7	0	4	-3*
-3	82	0	4	4	25	1	-2	-1	4	4	3*	1	32	1	0	-6	5	3	1*
-2	23	0	-2	5	11	1	2	0	24	1	1	2	14	1	1	-5	88	0	2
-1	72	1	-3	6	7	1	3*	1	10	2	2*	3	11	2	3*	-4	43	0	1
0	111	1	-10	H,K=		5,	3	H,K=		6,	-12	4	25	0	-3	-3	53	0	2
1	65	0	-4	-8	8	1	4	-6	7	8	-2*	H,K=		6,	-7	-2	79	0	1
2	34	0	-1	-7	25	1	1	-5	0	6	-1*	-9	26	0	0	-1	66	1	7
3	11	2	7*	-6	42	0	1	-4	3	7	-3*	-8	29	1	-2	0	16	1	7
4	62	1	11	-5	10	1	-2	-3	0	4	-4*	-7	40	1	-3	1	36	1	4
5	13	1	1	-4	8	2	2*	-2	9	1	4	-6	78	0	5	2	13	2	5
6	5	2	2*	-3	70	0	-5	-1	10	1	7	-5	52	0	3	3	20	1	-4
H,K=		5,	0	-2	7	2	-1*	H,K=		6,	-11	-4	17	2	2	4	21	0	7
-9	54	1	-0	-1	14	2	-3	-7	26	1	-2	-3	104	1	-6	5	18	2	-8

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF3 SB2F11

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		6,	-3	-2	48	0	-7	0	44	0	1	H,K=		7,	-8	4	5	7	3*
-10	24	1	-2	-1	22	0	1	1	0	5	-1*	-9	19	0	1	H,K=		7,	-4
-9	13	1	-1	0	25	1	0	2	12	1	-2	-8	23	0	1	-9	5	7	0*
-8	64	0	-5	1	9	1	6	3	29	0	3	-7	53	1	-3	-8	17	1	2
-7	34	1	-1	2	11	1	-6	H,K=		6,	5	-6	33	1	-7	-7	64	0	-2
-6	11	1	0	3	17	1	-6	-5	30	1	1	-5	22	1	1	-6	14	1	2
-5	76	0	6	4	0	4	-4*	-4	0	5	-3*	-4	33	1	1	-5	0	5	-2*
-4	0	6	-1*	5	4	5	-2*	-3	0	4	-0*	-3	22	0	-2	-4	37	1	2
-3	41	0	3	H,K=		6,	1	-2	35	1	-0	-2	38	0	-1	-3	6	1	4*
-2	117	1	-6	-8	34	0	-1	-1	3	4	1*	-1	35	0	-6	-2	19	1	4
-1	70	0	3	-7	12	1	-2	0	12	1	-2	0	22	0	-2	-1	22	0	-1
0	71	0	8	-6	24	1	-1	1	30	0	0	1	31	1	7	0	7	7	1*
1	36	0	2	-5	83	0	-1	2	10	2	3	2	27	1	-2	1	11	1	-6
2	62	0	4	-4	28	0	-5	H,K=		6,	6	3	6	6	0*	2	9	1	2
3	18	1	-2	-3	8	4	0*	-3	23	1	2	H,K=		7,	-7	3	1	8	-2*
4	13	1	5	-2	85	0	-5	-2	10	2	2*	-9	37	0	-5	4	7	3	6*
5	58	0	-6	-1	21	0	-4	-1	24	1	2	-8	26	1	-1	H,K=		7,	-3
H,K=		6,	-2	0	27	0	-1	0	31	0	4	-7	76	0	-2	-9	11	3	1*
-9	25	0	0	1	56	0	7	H,K=		7,	-12	-6	15	1	2	-8	30	0	-2
-8	68	0	-0	2	56	0	3	-6	8	5	-2*	-5	54	1	5	-7	87	0	-1
-7	7	2	-1*	3	13	1	-4	-5	17	1	-3	-4	61	0	1	-6	26	0	-4
-6	18	1	1	4	28	0	-5	-4	8	3	-3*	-3	27	0	-1	-5	10	1	0
-5	76	0	0	5	41	0	-3	-3	6	2	1*	-2	53	1	-6	-4	112	1	4
-4	21	1	-1	H,K=		6,	2	-2	18	1	1	-1	50	0	-2	-3	42	0	-2
-3	7	4	2*	-8	25	1	-1	H,K=		7,	-11	0	65	0	-2	-2	26	1	2
-2	74	1	-6	-7	38	0	-2	-7	20	1	-3	1	32	0	4	-1	96	1	-1
-1	43	0	3	-6	2	4	-2*	-6	10	1	-6	2	9	2	3*	0	64	0	2
0	15	2	7	-5	39	0	1	-5	62	0	-1	3	40	1	6	1	24	0	1
1	27	0	-1	-4	34	1	-1	-4	9	2	3	H,K=		7,	-6	2	31	1	7
2	19	1	2	-3	28	0	-3	-3	5	7	-2*	-9	12	2	-3	3	63	0	4
3	6	2	2*	-2	24	0	1	-2	54	1	-0	-8	21	1	-1	4	4	8	-1*
4	9	1	-1	-1	4	4	-1*	-1	4	4	-3*	-7	65	0	-2	H,K=		7,	-2
5	9	2	3	0	30	0	1	0	26	1	-1	-6	27	0	-2	-9	14	3	3
H,K=		6,	-1	1	7	1	-4*	H,K=		7,	-10	-5	28	0	2	-8	9	2	4
-9	26	1	-3	2	8	2	-1*	-8	6	3	5*	-4	39	0	2	-7	37	0	-2
-8	48	0	-2	3	29	0	3	-7	25	1	2	-3	29	0	1	-6	16	1	0
-7	22	1	-6	4	11	1	-6	-6	26	0	-4	-2	28	0	4	-5	9	1	1
-6	14	3	-2*	H,K=		6,	3	-5	27	1	-4	-1	28	0	-2	-4	31	0	-1
-5	102	1	5	-7	5	3	4*	-4	28	1	-5	0	20	0	1	-3	10	1	-2
-4	38	1	-4	-6	23	1	1	-3	10	1	-0	1	32	0	-0	-2	20	1	-3
-3	20	0	-5	-5	52	1	1	-2	35	0	-0	2	20	2	2	-1	6	2	5*
-2	110	1	-11	-4	1	6	-1*	-1	23	1	1	3	5	6	-4*	0	0	4	-2*
-1	35	0	-1	-3	9	2	-2*	0	12	2	3	4	11	2	3	1	14	2	-4
0	47	0	3	-2	64	0	-3	1	26	0	2	H,K=		7,	-5	2	5	7	-2*
1	59	0	-1	-1	9	1	1	H,K=		7,	-9	-9	25	0	-1	3	10	3	2*
2	68	0	3	0	14	2	1	-9	38	1	-2	-8	3	4	-6*	4	4	6	2*
3	11	1	-3	1	46	1	2	-8	36	0	-3	-7	84	0	-4	H,K=		7,	-1
4	24	1	5	2	36	1	5	-7	45	0	-0	-6	25	1	-2	-9	10	2	-3*
5	52	1	1	3	18	1	-2	-6	26	1	-3	-5	30	1	2	-8	31	1	-3
H,K=		6,	0	4	17	1	-0	-5	69	1	2	-4	96	1	7	-7	71	0	-2
-9	26	1	1	H,K=		6,	4	-4	38	0	-1	-3	57	0	-1	-6	9	1	-2
-8	50	0	-3	-6	11	1	1	-3	22	1	-1	-2	34	0	3	-5	7	1	2
-7	30	1	-1	-5	9	2	3*	-2	52	0	-0	-1	80	0	9	-4	96	0	-1
-6	8	4	-1*	-4	34	1	-0	-1	10	1	0	0	67	0	3	-3	26	0	-1
-5	54	0	3	-3	22	0	0	0	39	1	1	1	41	0	-1	-2	21	0	-6
-4	13	1	-1	-2	23	0	2	1	34	0	1	2	27	0	-2	-1	75	1	-6
-3	15	2	2	-1	22	0	2	2	6	2	-5*	3	60	0	1	0	40	0	-1

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF3 SB2F11

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	23	2	6	-1	5	3	2*	-1	36	0	-0	2	22	1	-1	H,K=		8,	3
2	44	1	2	0	19	1	-1	0	43	0	-2	3	14	3	1	-3	24	2	-1
3	54	1	-0	1	34	0	0	1	51	1	3	H,K=		8,	-2	-2	16	2	-2
4	14	1	-5	H,K=		8,-12		2	5	7	1*	-8	29	1	1	-1	28	0	-2
H,K=		7,	0	-4	35	1	-3	H,K=		8,	-6	-7	20	1	-3	H,K=		9,-11	
-8	8	2	4*	-3	14	1	-1	-9	26	1	-1	-6	5	9	-2*	-5	44	0	-3
-7	34	0	-3	H,K=		8,-11		-8	14	3	-4*	-5	28	0	-1	-4	28	1	-3
-6	37	0	-0	-7	38	1	-3	-7	0	6	-5*	-4	26	1	-2	-3	12	1	2
-5	24	0	-1	-6	34	1	-1	-6	17	1	1	-3	6	2	3*	H,K=		9,-10	
-4	5	2	3*	-5	9	1	1	-5	8	2	-1*	-2	14	1	3	-7	22	1	-2
-3	23	0	-4	-4	36	0	1	-4	18	1	3	-1	20	1	-3	-6	26	1	0
-2	25	0	-2	-3	22	1	1	-3	7	1	0	0	27	1	3	-5	3	4	3*
-1	5	2	3*	-2	23	1	-1	-2	6	1	4*	1	27	0	-0	-4	4	4	1*
0	10	2	2	-1	29	1	-1	-1	24	1	2	2	11	1	-5	-3	28	1	0
1	30	1	-1	H,K=		8,-10		0	5	6	-1*	3	15	1	4	-2	0	5	-5*
2	23	0	0	-8	23	1	-0	1	15	1	2	H,K=		8,	-1	-1	11	1	0
3	15	1	-3	-7	22	1	2	2	6	2	2*	-8	19	1	-2	H,K=		9,	-9
4	14	1	5	-6	20	0	-1	H,K=		8,	-5	-7	11	5	0*	-7	5	3	4*
H,K=		7,	1	-5	24	2	-6	-9	63	1	-3	-6	65	0	-2	-6	13	1	1
-8	28	1	-1	-4	42	0	-4	-8	15	1	3	-5	14	1	1	-5	70	0	-3
-7	41	0	-2	-3	24	1	-2	-7	16	1	-2	-4	8	2	-1*	-4	33	0	-2
-6	13	2	-2	-2	8	1	3	-6	104	1	-1	-3	61	1	-7	-3	15	2	-1
-5	13	1	-1	-1	30	2	1	-5	15	2	1	-2	11	4	-1*	-2	37	0	-5
-4	67	0	-3	0	16	2	-3	-4	16	1	3	-1	28	1	-1	-1	33	1	-4
-3	4	5	2*	H,K=		8,	-9	-3	93	1	6	0	39	1	3	0	5	8	1*
-2	13	2	0	-8	18	2	-1	-2	47	0	1	1	25	1	5	H,K=		9,	-8
-1	51	0	1	-7	27	0	-1	-1	32	0	-1	2	33	1	-4	-8	0	8	-1*
0	26	1	-1	-6	71	0	-2	0	48	0	4	3	7	2	-7*	-7	11	1	0
1	31	0	1	-5	10	1	1	1	56	1	6	H,K=		8,	0	-6	8	2	3*
2	36	0	-1	-4	35	0	-3	2	12	1	1	-7	17	1	-2	-5	14	1	1
3	32	1	2	-3	43	1	-4	3	13	1	1	-6	2	4	-1*	-4	2	5	-2*
H,K=		7,	2	-2	41	0	-2	H,K=		8,	-4	-5	33	0	-1	-3	16	1	0
-7	10	1	-0	-1	23	0	4	-9	9	1	1	-4	33	0	-4	-2	13	1	0
-6	40	1	-2	0	17	1	2	-8	10	1	-1	-3	17	2	-0	-1	20	2	-0
-5	21	1	-2	1	37	2	-1	-7	13	2	-4	-2	25	1	-0	0	15	3	3*
-4	0	7	-7*	H,K=		8,	-8	-6	17	1	0	-1	20	1	3	H,K=		9,	-7
-3	30	0	0	-9	23	1	5	-5	9	1	3	0	20	0	2	-8	67	0	-1
-2	32	0	-3	-8	21	2	-4	-4	5	2	-2*	1	20	1	1	-7	0	8	-9*
-1	8	1	1	-7	25	1	-1	-3	10	1	0	2	18	1	3	-6	7	1	7
0	27	0	-3	-6	29	0	-2	-2	15	1	-5	H,K=		8,	1	-5	83	0	2
1	35	0	6	-5	31	1	-4	-1	2	4	2*	-6	37	0	-2	-4	25	1	-2
2	15	1	-0	-4	26	0	1	0	10	1	8	-5	28	0	-3	-3	24	0	-4
3	13	1	2	-3	15	1	-1	1	19	1	3	-4	7	1	2*	-2	54	0	-1
H,K=		7,	3	-2	6	1	2*	2	5	5	1*	-3	39	0	1	-1	37	1	1
-6	19	0	1	-1	32	0	5	3	14	2	-1	-2	0	5	-5*	0	9	1	-1
-5	6	2	-3*	0	12	1	-1	H,K=		8,	-3	-1	34	0	0	1	23	1	-0
-4	41	1	-1	1	8	2	2*	-9	58	0	-4	0	25	1	-3	H,K=		9,	-6
-3	10	2	-4*	2	19	1	2	-8	14	2	1	1	4	5	0*	-8	1	7	-1*
-2	15	1	-0	H,K=		8,	-7	-7	22	1	0	2	30	2	-2	-7	0	5	-3*
-1	34	0	2	-9	56	0	0	-6	91	1	0	H,K=		8,	2	-6	9	2	-2*
0	3	5	1*	-8	11	3	-0*	-5	3	4	-2*	-5	33	1	-0	-5	33	1	-0
1	29	1	0	-7	9	1	4	-4	15	2	-3	-4	24	1	-3	-4	16	1	-3
2	21	1	-2	-6	101	0	-4	-3	86	1	-11	-3	4	7	-3*	-3	6	3	4*
H,K=		7,	4	-5	25	0	1	-2	27	1	1	-2	25	0	0	-2	20	0	-0
-4	8	3	4*	-4	21	0	-4	-1	21	1	1	-1	23	1	2	-1	26	1	5
-3	29	1	1	-3	64	0	-0	0	42	1	4	0	12	1	1	0	5	2	-1*
-2	26	1	3	-2	41	0	-5	1	47	0	1	1	12	1	-1	1	19	1	1

OBSERVED STRUCTURES FACTORS (CONT) FOR
XEF3 S82F11

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		9,	-5	-1	21	1	-1	-5	15	5	-2*								
-8	64	1	-2	0	10	2	3*	-4	18	1	-3								
-7	12	1	3	H,K=		9,	1	-3	10	2	-1								
-6	7	2	1*	-4	32	1	-3	-2	2	6	-1*								
-5	84	0	3	-3	31	1	-2												
-4	7	3	1*	-2	10	2	-1*												
-3	24	1	-1	-1	15	1	-3												
-2	49	1	-0	H,K=		10,	-9												
-1	33	1	-2	-6	13	2	-3												
0	19	1	0	-5	6	7	-4*												
1	20	1	1	-4	48	0	-3												
H,K=		9,	-4	-3	21	2	-2												
-8	20	1	-1	H,K=		10,	-8												
-7	23	1	-2	-6	13	3	-1*												
-6	23	1	-1	-5	4	8	-0*												
-5	19	1	1	-4	33	1	2												
-4	14	1	-0	-3	13	1	0												
-3	13	1	-4	-2	13	1	1												
-2	32	0	-3	H,K=		10,	-7												
-1	36	0	-1	-7	53	1	0												
0	11	1	-3	-6	0	4	-5*												
1	25	1	10	-5	14	2	-0												
H,K=		9,	-3	-4	54	1	2												
-8	48	0	0	-3	15	1	-2												
-7	23	2	1	-2	23	1	0												
-6	8	1	-3	-1	24	1	2												
-5	65	1	-4	H,K=		10,	-6												
-4	11	1	-3	-7	35	1	-2												
-3	23	1	-6	-6	20	1	-1												
-2	36	1	-3	-5	9	2	-1*												
-1	12	1	0	-4	39	0	-2												
0	31	0	-1	-3	20	1	-2												
1	17	1	-2	-2	5	3	4*												
H,K=		9,	-2	-1	28	0	3												
-7	26	1	0	H,K=		10,	-5												
-6	25	1	0	-7	45	1	-0												
-5	20	0	1	-6	17	1	2												
-4	16	1	0	-5	20	1	-1												
-3	20	1	-5	-4	41	0	-2												
-2	27	1	-2	-3	0	4	-1*												
-1	29	1	3	-2	30	1	-1												
0	16	1	-2	-1	12	3	-1*												
1	22	1	-0	H,K=		10,	-4												
H,K=		9,	-1	-6	20	1	-0												
-6	7	3	-3*	-5	21	1	1												
-5	37	1	-1	-4	28	0	-3												
-4	24	0	-3	-3	13	1	-1												
-3	30	1	-3	-2	9	2	1												
-2	27	2	-2	-1	28	1	5												
-1	2	5	-3*	H,K=		10,	-3												
0	39	1	-1	-6	27	1	-3												
1	14	1	1	-5	19	2	-3												
H,K=		9,	0	-4	30	1	-7												
-5	13	1	1	-3	16	1	1												
-4	18	2	1	-2	36	0	-2												
-3	17	1	-1	-1	8	2	0												
-2	18	2	-1	H,K=		10,	-2												

TABLE III

Interatomic Distances (Å) and Angles (Deg.) for $XeF_3^+Sb_2F_{11}^-$
(Standard Deviations 0.01 Å for all Distances)

Intramolecular Distances		Intramolecular Angles		Intermolecular Distances (≤ 3.5 Å)	
Xe-F(2)	2.50	F(1)-Sb(2)-F(4)	85.80(27)	Xe-F(3)[b]	2.97
F(9)	1.83	F(6)	86.30(30)	F(4)[j]	3.17
F(10)	1.88	F(7)	178.81(37)	F(7)[c]	3.04
F(11)	1.89	F(13)	85.07(25)	F(8)[e]	3.26
Sb(1)-F(1)	2.01	F(14)	84.56(26)	F(13)[b]	2.94
F(2)	1.90	F(2)-Sb(1)-F(1)	85.60(25)	F(1)-F(5)[f]	2.91
F(3)	1.85	F(3)	86.26(32)	F(10)[e]	3.34
F(5)	1.84	F(5)	171.94(37)	F(11)[b]	3.28
F(8)	1.85	F(8)	91.24(31)	F(2)-F(3)[b]	3.17
F(12)	1.83	F(12)	89.10(33)	F(8)[e]	3.03
Sb(2)-F(1)	2.04	F(3)-Sb(1)-F(1)	85.24(29)	F(10)[e]	3.24
F(4)	1.86	F(5)	90.78(34)	F(13)[b]	2.91
F(6)	1.84	F(8)	95.29(35)	F(3)-F(3)[b]	3.40
F(7)	1.85	F(12)	169.26(46)	F(7)[k]	3.27
F(13)	1.86	F(4)-Sb(2)-F(6)	89.09(36)	F(11)[b]	2.78
F(14)	1.86	F(7)	93.58(31)	F(13)[b]	3.27
F(1)-F(2)	2.66	F(13)	88.91(32)	F(14)[b]	2.84
F(3)	2.62	F(14)	170.35(38)	Xe[b]	2.97
F(4)	2.66	F(5)-Sb(1)-F(1)	86.69(27)	F(4)-F(4)[d]	3.45
F(5)	2.65	F(8)	96.50(32)	F(5)[f]	3.02
F(6)	2.66	F(12)	92.52(37)	F(9)[g]	3.00
F(13)	2.64	F(6)-Sb(2)-F(7)	94.70(32)	F(11)[b]	3.30
F(14)	2.63	F(13)	171.27(48)	F(11)[g]	2.77
F(2)-F(3)	2.56	F(14)	90.70(36)	F(12)[f]	3.48
F(8)	2.68	F(7)-Sb(2)-F(13)	93.91(34)	F(5)-F(5)[f]	3.06
F(10)	2.64	F(14)	96.05(32)	F(6)[k]	3.06
F(12)	2.62	F(8)-Sb(1)-F(1)	176.76(36)	F(6)[f]	3.47
F(14)	3.07	F(12)	94.49(39)	F(9)[m]	3.23
F(3)-F(5)	2.63	F(9)-Xe-F(10)	81.73(30)	F(11)[b]	3.00
F(8)	2.74	F(11)	80.22(30)	F(12)[f]	3.40
F(13)	3.09	F(2)	154.39(38)	F(6)-F(6)[a]	2.98
F(4)-F(6)	2.59	F(10)-Xe-F(11)	161.90(40)	F(8)[r]	3.12
F(7)	2.71	F(2)	72.67(27)	F(9)[e]	3.08
F(13)	2.61	F(11)-Xe-F(2)	125.34(31)	F(9)[g]	3.39
F(5)-F(8)	2.76	F(12)-Sb(1)-F(1)	84.76(29)	F(10)[e]	2.89
F(12)	2.65	F(13)-Sb(2)-F(14)	89.84(33)	F(7)-F(9)[c]	2.99
F(6)-F(7)	2.71	Sb(1)-F(1)-Sb(2)	155.37(15)	F(9)[g]	3.18
F(14)	2.63	Xe-F(2)-Sb(1)	171.64(13)	F(11)[g]	3.31
F(7)-F(13)	2.71			F(11)[c]	3.29
F(14)	2.76			F(12)[n]	3.04
F(8)-F(13)	2.70			F(14)[c]	3.12
F(9)-F(10)	2.43			F(8)-F(8)[s]	3.19
F(11)	2.40			F(10)[s]	2.95
F(13)-F(14)	2.63			F(13)[b]	3.50
				F(9)-F(9)[t]	3.32
				F(11)[t]	2.83
				F(12)[e]	2.94
				F(10)-F(10)[e]	2.67
				F(12)[c]	3.15
				F(14)[e]	3.06
				F(11)-F(12)[p]	3.25
				F(13)[b]	2.85
				F(12)-F(13)[q]	3.25
				F(14)-F(14)[c]	3.01

References for Table III: Interatomic Distances (Å)and Angles for $XeF_3^+Sb_2F_{11}^-$.

*The crystal-chemical unit is at x,y,z and the letters refer to positions:

a(-x,-y,-z); b(1-x,1-y,-z); c(1-x,1-y,-z); d(1-x,-y,1-z); e(-x,1-y,-z);

f(-x,-y,1-z); g(-x,-1-y,-1-z); h(1-x,-y,-z); i(1-x,2-y,-z);

j(x,1+y,z); k(x,y,1+z); ℓ(x,-1+y,z); m(x,-1+y,1+z); n(1+x,y,z);

p(1+x,1+y,z); q(-1+x,y,z); r(x,y,-1+z); s(-x,1-y,1-z).

TABLE IV

Comparison of ClF_3, BrF_3 and XeF_3^+

	ClF_3	BrF_3	XeF_3^+
$E\text{-}F_{equatorial}$ (Å)	1.598	1.721	1.83
$E\text{-}F_{axial}$ (Å)	1.698	1.810	1.88, 1.89
$F_{ax}E\text{-}F_{eq}$	87.5°	86.2°	82, 80
Reference	10	11	present work

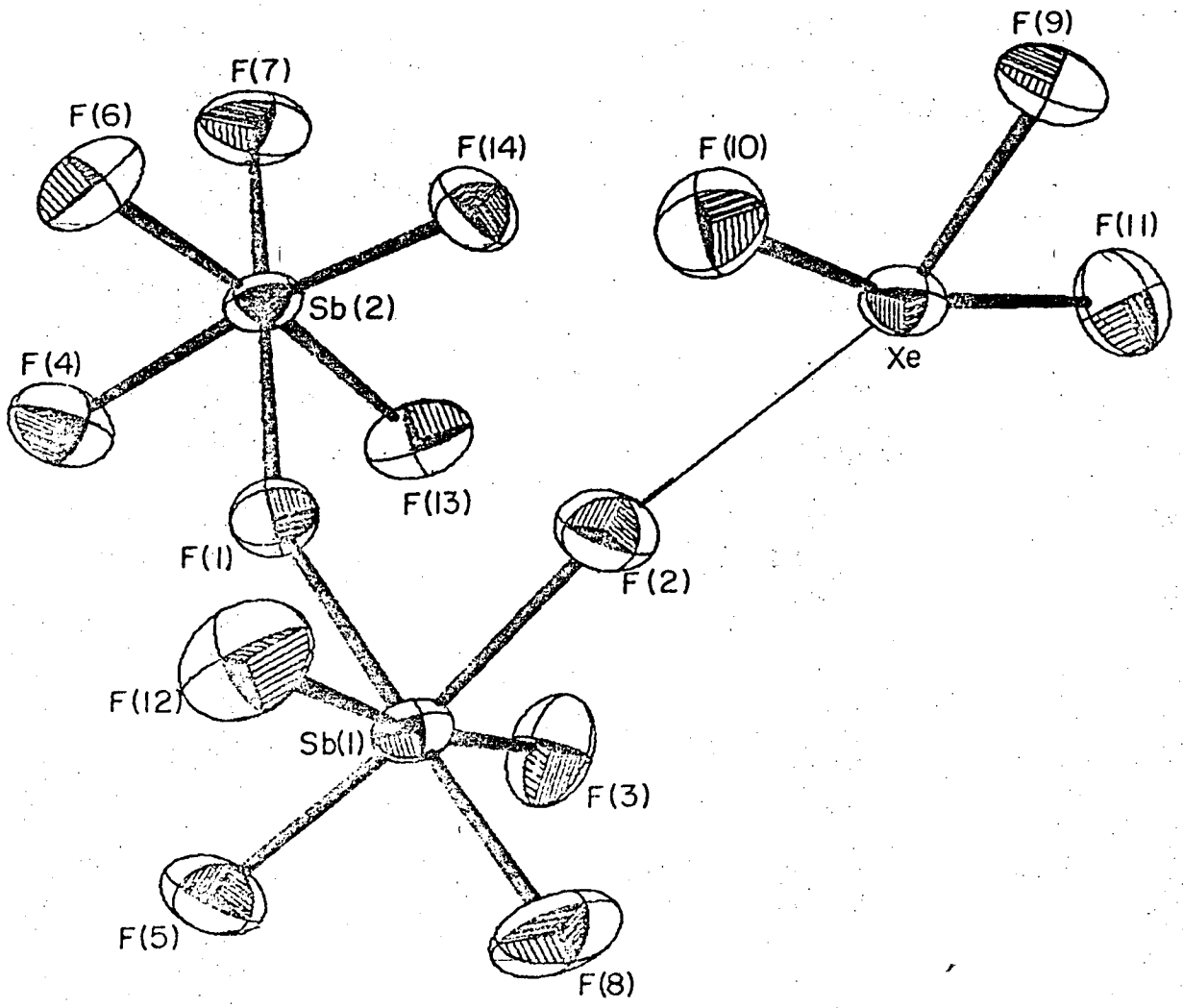

Figure 1(a): The structural unit $XeF_3^+Sb_2F_{11}^-$

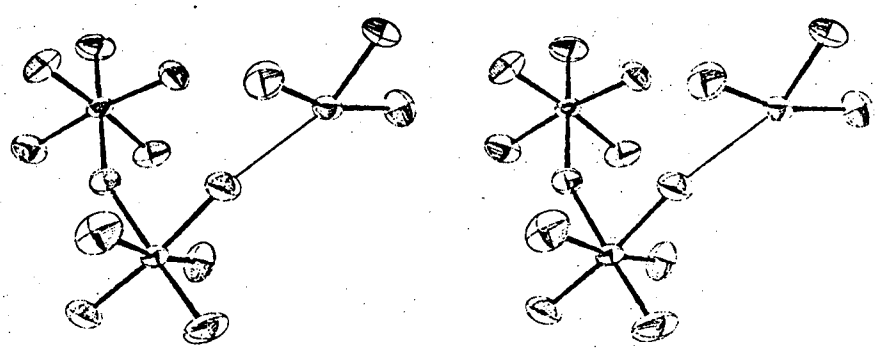

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Figure 1(b): Stereogram of the $XeF_3^+Sb_2F_{11}^-$ structural unit.

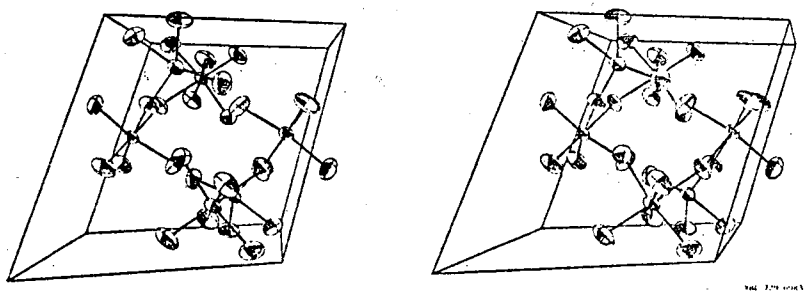

Figure 2: Stereogram showing the arrangement of the $XeF_3^+Sb_2F_{11}^-$ structural units within the unit cell - view along b.

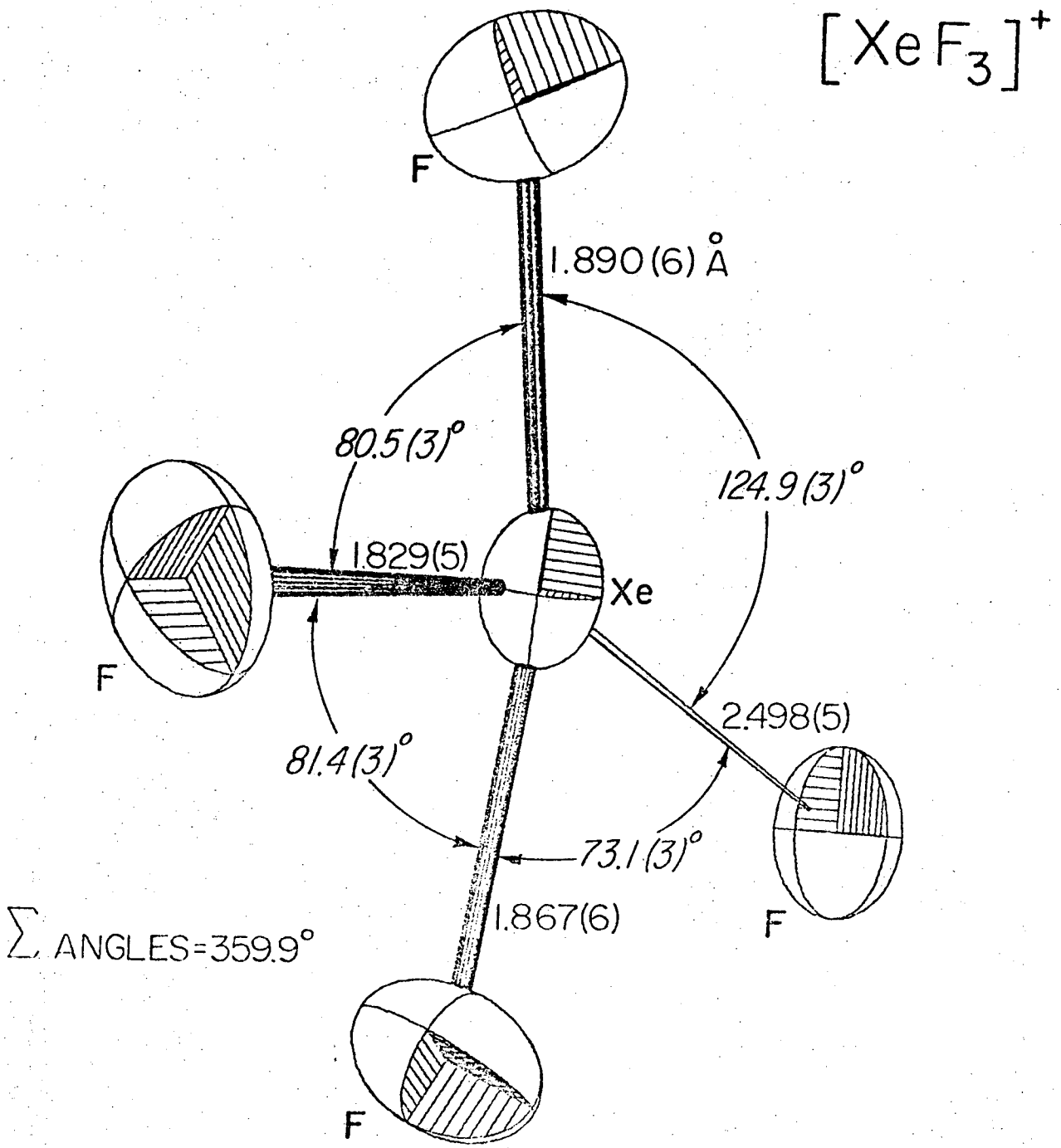

Figure 3: The XeF_3^+ ion and its close contact with the $Sb_2F_{11}^-$ ion.

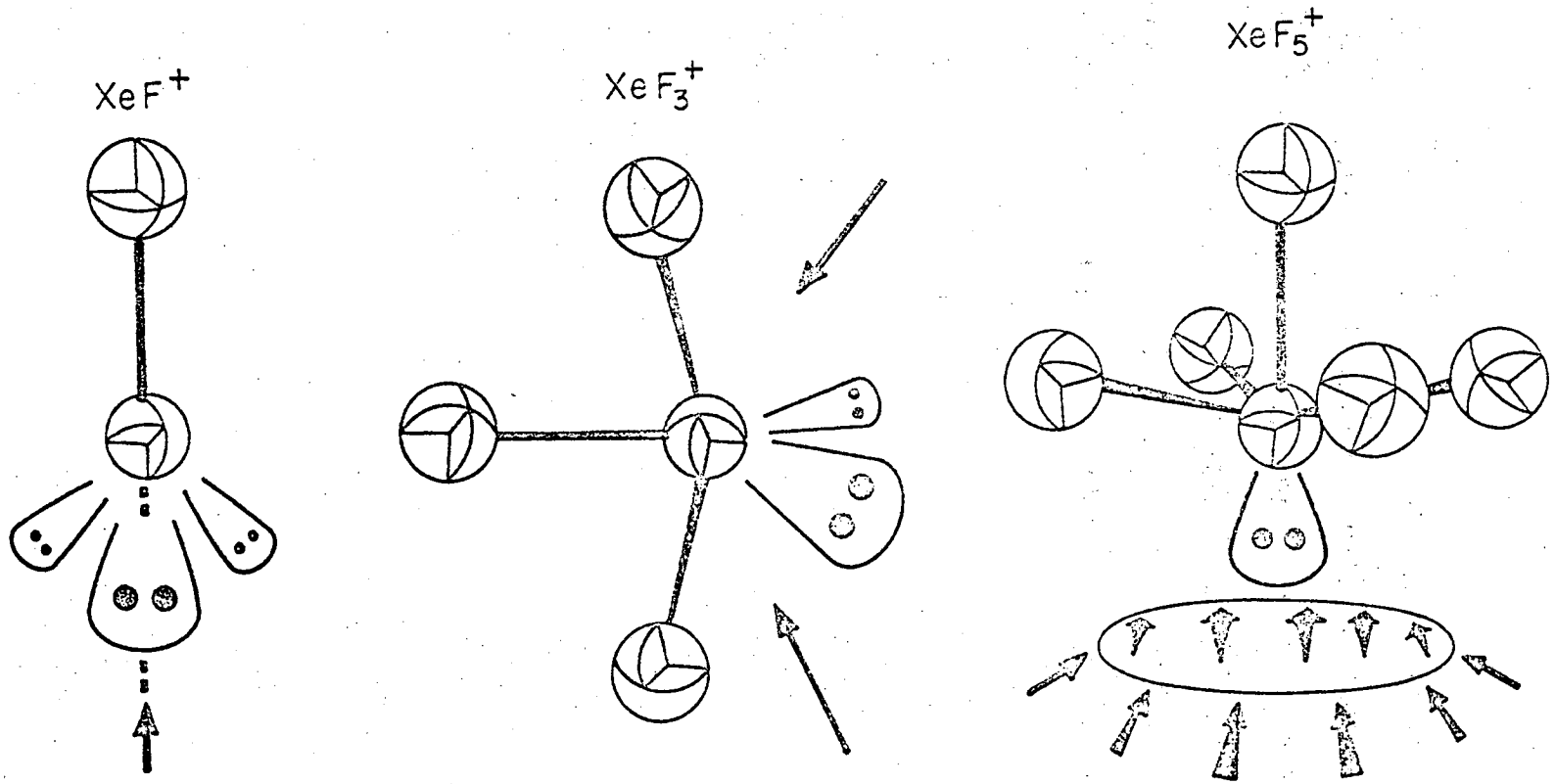

Figure 4: Shapes of the XeF_x^+ ions based on steric activity of the non-bonding xenon valence electron pairs. (Arrows indicate directions of maximum polarizing effect.)

Footnote for Figure 4:

These models represent the non-bonding xenon electrons in a formalistic way. In the $Xe\text{-}F^+$ case the model cannot be realistic since such a cation has cylindrical symmetry. The postulated axial polarizing behaviour can also be seen to be a consequence of Xe-F bond formation. Thus we can "synthesize" $(XeF)^+$ by bringing $F^+(^1D)$ up to the spherical Xe atom. If we use a p orbital pair of electrons of the Xe atom to form the Xe-F bond, the electron density will be diminished trans to the bond.

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