Crystal Structure of Na₃Sr₄Al₅F₂₆

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Na₃Sr₄Al₅F₂₆ is tetragonal (space group $P4_2/n$) with a = 10.2679(5) Å, c = 18.373(2) Å, and Z = 4. The structure is refined, despite a systematic twinning, from 1478 reflections to $R_F = 0.029$ ($R_1 = 0.039$). Aluminum ions are in octahedral sites while strontium and sodium atoms are respectively in nine- and eightfold coordination. The structure is characterized by isolated $[Al_5F_{26}]^{1/2}$ pentamers. A distorted cube $[Na_{(1)}F_8]^{7-}$ ensures the connection between the octahedra pentamers and builds up $[NaAl_5F_{26}]^{10-}$ chains running along the *b*-axis at level z = 0 and along the *a*-axis at level $z = \frac{1}{2}$. Strontium (Sr₍₁₎ and Sr₍₂₎) and sodium (Na₍₂₎ and Na₍₃₎) are inserted between the chains. @ 1989 Academic Press, Inc.

Introduction

The investigation of the ternary system NaF-SrF₂-AlF₃ by means of the chloride flux method (1, 2) has evidenced three new phases: two fluorides NaSrAlF₆ (3) on Na₃Sr₄Al₅F₂₆ and a chlorofluoride Sr₁₀Al₂ F₂₅Cl (4). We present here the crystal structure of Na₃Sr₄Al₅F₂₆ from single-crystal data.

Preparation

Crystals of Na₃Sr₄Al₅F₂₆ were synthesized using a chloride flux method in a platinum crucible under argon atmosphere. They are obtained from the mixture NaF + 2SrF₂ + 2AlF₃ + 4.5NaCl + 2.75ZnCl₂ by slow cooling (6°C/hr) from 700°C. Na₃Sr₄Al₅F₂₆ crystals, with a stretched octahedron or plate habit (<1 mm³), are obtained with a small amount of two other phases: NaSrAlF₆ (3) and an unknown compound whose diffraction pattern is very close to that of Jarlite—Na₄Sr₁₂Mg₂ Al₁₂F₆₄(OH)₄ (5).

The solid-state synthesis of $Na_3Sr_4Al_5F_{26}$ has been achieved, in sealed gold tubes, at 650°C (40 hr) from a stoichiometric mixture of elementary fluorides.

Structural Determination of Na₃Sr₄Al₅F₂₆

The crystal selected for X-ray data collection on a Siemens AED2 four-circle diffractometer has an approximate volume of 1.75×10^{-3} mm³ and is limited by faces (100, 010, 001). The lattice parameters—a= 10.2679(5) Å, c = 18.373(2) Å—were refined from 40 reflections by a double-scan technique. The conditions of the diffraction experiment are summarized in Table I.

The observed reflection conditions hk0, h + k = 2n, and 00l, l = 2n—lead to the space group $P4_2/n$. Intensities, corrected from Lorentz—polarization effects as well as for absorption using the correct

TABLE	l
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Crystal Data and Conditions of Data Collection and Refinement for $Na_3Sr_4Al_5F_{26}$

Symmetry	Tetragonal
Space group	$P4_2/n$ (No. 86)
Cell parameters	a = 10.2679(5) Å,
	c = 18.373(2) Å;
	$V = 1937.06 \text{ Å}^3; Z = 4$
Crystal volume (10 ⁻³ mm ³)	1.75
Radiation	Mo Kα (graphite mono- chromatized)
Scanning mode	$\omega/2\theta$
Aperture (mm)	3/3
Range registered	
$\theta_{\min}, \ \theta_{\max}$ (°)	2.00, 30.00
h, k, l max	14, 10, 25
Absorption coefficient μ (cm ⁻¹)	111.54
Absorption correction	Gaussian method
Transmission factors	max: 0.4339
	min: 0.2417
Reflections measured:	
Total	6359
Independent (R _{average})	2764, ($R = 0.024$) in $4/m$
	1696, $(R = 0.026)$ in 4/mmm
Used in refinement	2409 ($F_{\rm o} > 6\sigma(F_{\rm o})$) in $4/m$
	1478 ($F_{o} > 6\sigma(F_{o})$) in $4/mmm$
Number of refined pa-	75 (with isotropic ther-
rameters	mal parameters)
	176 (with anisotropic
	thermal parameters)
Reliability factor	$R_{\rm F} = (\sum F_{\rm o} - k F_{\rm c} / \sum F_{\rm o})$
	$R_{\rm I} = (\Sigma I_{\rm o} - kI_{\rm c} / \Sigma I_{\rm o})$

final composition, were averaged in Laue group 4/m and led to an R_{av} value of 0.024.

In the first trial, the structure refinement was performed using the SHELX76 program (6). Ionic scattering factors and anomalous dispersion parameters were taken from "International Tables for X-Ray Crystallography" (7). The structure was solved from the TANG option of direct methods in the space group $P4_2/n$. Two strontium sites (8g) and one aluminum site (4c) were first located; this led to a reliability factor $R_F = 0.42$. From successive difference Fourier maps and refinements, the other atoms were easily located but the final R_F value decreased only to 0.21 with isotropic thermal motion. At this stage of refinement the structural formulation obtained was Na₃Sr₄Al₅F₂₆ and no new peaks were observed in the difference Fourier map. Moreover all the Al-F, Na-F, and Sr-F distances are realistic. The failure of the structure refinement compelled us to assume a twinning process, involving an increase of the Laue symmetry.

Indeed, when looking at the structure factors for pairs of reflections hk0/kh0 and hkl/khl, it appears that the observed F_o obey the Laue symmetry 4/mmm instead of 4/m. Thus, if the space group $P4_2/n$ is the correct one, there is only one solution to this problem: two domains, with a volume ratio near unity, which superpose their hkl and khl reflections.

A structure refinement with the only reflections unaffected by the twinning (*hhl* and *h0l*) and isotropic temperature factors converges to $R_F = 0.06$ (406 *hkl*, 75 refined parameters). This confirms the suggested twin model for our crystal.

In order to solve the structure with a twinned crystal (a limited data collection of two other crystals shows the same twinning) the observed intensities were merged in the 4/mmm Laue group ($R_{av} = 0.026$ for 1696 hkl). Each observed intensity (I_0) was considered to result from two domains (A and B) with equal volume according to the expression $I_0 = I_{hklA} + I_{khlB}$. For calculation we have used a local program (unpublished) where the minimized function was χ^2 = $\sum w_i (I_o - kI_c)^2$ with $I_c = F_{hklA}^2 + F_{khlB}^2$, $w_i =$ $1/I_0$ (ponderation scheme) and k = scale factor. Starting from the atomic positions previously obtained, and refining with isotropic temperature factors, the reliability factor fell to $R_{\rm F} = 0.054$ ($R_{\rm I} = 0.069$) and further to $R_{\rm F} = 0.029 \ (R_{\rm I} = 0.039)$ when applying anisotropic thermal motion. This

A1	OMIC	PARAMETE	RS, ANISO	ROPIC LEM	PERATUR	E FACIO	$RS^{u} U_{ij} \times$	IU" AND B	₂₉ (A ²) FOI	$R Na_3 Sr_4 AI_5$	F ₂₆
Atom	Site	x	у	z	<i>U</i> 11	U ₂₂	U_{33}	U_{12}	U_{13}	U_{23}	Beq
Sr ₁	8g	0.2821(0)	0.9974(1)	0.8254(0)	59(0)	75(0)	152(0)	-8(0)	-14(0)	-14(0)	0.75
Sr ₂	8g	0.2873(0)	0.9970(1)	0.1944(0)	66(0)	72(0)	84(0)	-12(0)	16(0)	-9(0)	0.58
Al_1	4c	0	0	0	112(11)	48(11)	77(0)	~112(21)	9(9)	-3(9)	0.62
Al_2	8g	0.5155(2)	0.7555(2)	0.8727(1)	5(11)	64(5)	65(0)	-4(5)	18(9)	1(9)	0.35
Al ₃	8g	0.2523(2)	0.5098(3)	0.6339(1)	48(5)	101(11)	73(0)	0(5)	4(9)	19(9)	0.59
Na_1	4d	0	0	$\frac{1}{2}$	181(21)	438(27)	188(17)	-107(48)	29(19)	-124(19)	2.12
Na_2	4f	$\frac{1}{4}$	$\frac{1}{4}$	0.9978(0)	192(43)	389(48)	68(17)	262(32)	0	0	1.71
Na_3	4e	<u>3</u> 4	$\frac{1}{4}$	0.9959(3)	25(48)	763(80)	154(34)	-171(48)	0	0	3.07
\mathbf{F}_{1}	8g	0.1266(4)	0.0093(6)	0.7056(2)	117(16)	139(21)	120(17)	11(21)	38(9)	3(19)	0.99
\mathbf{F}_2	8g	0.3361(6)	0.1192(6)	0.6710(3)	160(27)	246(32)	291(34)	-91(21)	0(29)	-86(29)	1.83
\mathbf{F}_3	8g	0.6673(6)	0.1132(5)	0.6720(3)	165(27)	133(27)	171(17)	59(21)	1(19)	-9(19)	1.24
F4	8g	0.3232(5)	0.8760(6)	0.6947(3)	192(27)	165(27)	137(17)	80(21)	-57(19)	29(19)	1.30
F_5	8g	0.4513(5)	0.3695(5)	0.0602(3)	176(27)	149(21)	188(17)	-37(21)	-9(19)	96(19)	1.35
F_6	8g	0.1392(5)	0.3560(5)	0.0879(2)	139(27)	128(27)	103(17)	-59(16)	9(19)	3(19)	0.97
\mathbf{F}_7	8g	0.3630(5)	0.8513(5)	0.0943(2)	149(27)	117(27)	120(17)	37(16)	-57(19)	-38(19)	1.02
F_8	8g	0.5031(6)	0.1226(4)	0.1975(2)	117(21)	80(16)	120(17)	37(21)	-7(19)	38(9)	0.83
F9	8g	0.1574(4)	0.9958(6)	0.9636(2)	112(16)	203(21)	171(17)	11(21)	29(19)	2(19)	1.28
\mathbf{F}_{10}	8g	0.3951(5)	0.8402(5)	0.9255(3)	80(27)	171(27)	154(17)	11(21)	57(19)	-9(19)	1.06
$\mathbf{F}_{\mathbf{H}}$	8g	0.3742(5)	0.9537(6)	0.5661(3)	128(21)	208(27)	171(17)	5(16)	95(19)	-9(19)	1.33
\mathbf{F}_{12}	8g	0.3429(5)	0.3968(6)	0.5786(2)	149(27)	181(27)	137(17)	59(21)	29(19)	-38(19)	1.23
F_{13}	8g	0.3728(6)	0.3242(5)	0.1872(2)	155(27)	160(27)	137(17)	80(21)	-7(19)	-38(19)	1.19

TABLE II

Note. Numbers in parentheses indicate esd's.

^a The vibrational coefficients relate to the expression: $T = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + l^2c^{*2}U_$ $2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})].$

result, obtained without any major deviation for the atomic coordinates, well confirms the twinning of our crystal. Table II lists the positional and thermal motion parameters and Table III gives the main interatomic distances and angles. A table of I_0 and I_c can be obtained on request to the authors.

Structure Description

The main feature of the Na₃Sr₄Al₅F₂₆ structure corresponds to the existence of isolated pentamers [Al₅F₂₆]¹¹⁻ built up from five aluminum octahedra. In these pentamers (Fig. 1) the central $Al_{(1)}$ octahedron is corner-connected to four other octahedra in such a way that the $Al_{(2)}$ octahedra (and also Al₍₃₎) are always in *trans*-position. These entities are parallel to the (b, c) plane

at level z = 0 and are rotated by 90° around the *c*-axis at level $z = \frac{1}{2}$ (Fig. 2).

The sodium and strontium atoms are respectively in eight- and ninefold coordination. The NaF₈ (Na₁) polyhedron, which looks like a distorted cube, is also shown in Fig. 1. These polyhedra establish the connection between the $[Al_5F_{26}]^{11-}$ blocks and build up [NaAl₅F₂₆]¹⁰⁻ chains running either along the *b*-axis at level z = 0 (Fig. 3) or along the *a*-axis at level $z = \frac{1}{2}$ (Fig. 4). The



FIG. 1. Perspective view of [Al₅F₂₆]¹¹⁻ pentamers and [Na₍₁₎F₈]⁷⁻ polyhedra.

TABLE III

Main Interatomic Distances (Å) and Angles (°) in $NaSr_4Al_5F_{26}{}^a$

$\begin{split} Sr_1^{2+} \text{ polyhedron [9]} \\ Sr_1-F_2 &= 2.393(6) \\ Sr_1-F_3 &= 2.422(6) \\ Sr_1-F_1 &= 2.581(4) \\ Sr_1-F_1 &= 2.2681(5) \\ Sr_1-F_1 &= 2.722(3) \\ Sr_1-F_1 &= 2.722(3) \\ Sr_1-F_4 &= 2.737(5) \\ Sr_1-F_7 &= 2.844(3) \\ \langle Sr_2-F_4 &= 2.449(6) \\ Sr_2-F_1 &= 2.449(6) \\ Sr_2-F_1 &= 2.449(6) \\ Sr_2-F_1 &= 2.449(6) \\ Sr_2-F_3 &= 2.449(6) \\ Sr_2-F_1 &= 2.449(6) \\ Sr_2-F_3 &= 2.468(6) \\ Sr_2-F_1 &= 2.268(2) \\ Sr_2-F_1 &= 2.268(2) \\ Sr_2-F_1 &= 2.268(2) \\ Sr_2-F_1 &= 2.682(2) \\ Sr_2-F_3 &= 2.268(2) \\ Sr_2-F_1 &= 2.618(5) \\ Sr_2-F_1 &= 2.268(2) \\ Al_1-F_1 &= 2 \times 1.836(3) \\ F_9-Al_1-F_{11} &= 2 \times 90.2(4) \\ F_9-F_1 &= 2.5212(6) \\ Al_1-F_1 &= 2 \times 1.836(3) \\ F_9-Al_1-F_{11} &= 2 \times 87.4(5) \\ F_3-Al_1-F_{11} &= 2 \times 92.6(5) \\ F_3-F_1 &= 2.634(7) \\ Al_1-F_1 &= Al_2 &= 152.8(1) \\ Al_1-F_1 &= Al_2 &= 153.2(3) \\ \hline Al_2^{1+} \text{ octahedron} \\ Al_2-F_1^* &= 1.788(4) \\ Al_2-F_1^* &= 1.801(3) \\ Al_3-F_1^* &= 1.801(3) \\ Al_3-F_1^* &= 1.801(3) \\ Al_3-F_1^* &= 1.801(3) \\ Al_3-F_1^* &= 1.802(3) \\ \hline \end{pmatrix}$			
$\begin{split} Sr_1-F_2 &= 2.393(6)\\ Sr_1-F_3 &= 2.422(6)\\ Sr_1-F_1 &= 2.283(4)\\ Sr_1-F_1 &= 2.283(4)\\ Sr_1-F_1 &= 2.709(5)\\ Sr_1-F_1 &= 2.709(5)\\ Sr_1-F_1 &= 2.727(5)\\ Sr_1-F_4 &= 2.737(5)\\ Sr_1-F_4 &= 2.737(5)\\ Sr_1-F_5 &= 2.844(3)\\ (Sr_1-F) &= 2.628\\ \hlinelabel{eq:starsec} \\ Sr_2-F_1 &= 2.494(6)\\ Sr_2-F_1 &= 2.494(6)\\ Sr_2-F_1 &= 2.494(6)\\ Sr_2-F_1 &= 2.284(2)\\ Sr_2-F_6 &= 2.582(2)\\ Sr_2-F_6 &= 2.582(2)\\ Sr_2-F_6 &= 2.584(8)\\ Sr_2-F_6 &= 2.584(8)\\ Sr_2-F_1 &= 2.628(2)\\ Sr_2-F_6 &= 2.584(8)\\ Sr_2-F_7 &= 2.263(5)\\ Sr_2-F_1 &= 2.263(6)\\ Sr_2-F_7 &= 2.263(6)\\ Sr_2-F_7 &= 2.263(6)\\ Al_1-F_5 &= 2.8136(3)\\ F_9-Al_1-F_{11} &= 2.89.8(4)\\ F_9-F_1 &= 2.531(6)\\ (Al_1-F) &= 1.798\\ F_9-Al_1-F_{11} &= 2.89.8(4)\\ F_9-F_{11} &= 2.531(6)\\ F_5-Al_1-F_{11} &= 2.89.8(4)\\ F_2-F_{11} &= 2.531(6)\\ F_5-Al_1-F_{11} &= 2.89.8(4)\\ F_2-F_{11} &= 2.531(6)\\ F_3-Al_1-F_{11} &= 2.89.8(4)\\ F_2-F_{11} &= 2.531(6)\\ F_3-Al_1-F_{11} &= 2.89.8(4)\\ F_3-F_{11} &= 2.531(6)\\ F_3-Al_2 &= 153.2(3)\\ \hlinelabel{eq:starsec} Al_2^{24} &= 153.2(3)\\ \hlinelabel{eq:starsec} Al_2^{24} &= 153.2(3)\\ \hlinelabel{eq:starsec} Al_3^{24} &= 1.788(4)\\ Al_2-F_1^* &= 1.801(4)\\ Al_2-F_1^* &= 1.801(4)\\ Al_2-F_1^* &= 1.801(4)\\ Al_2-F_1^* &= 1.801(3)\\ Al_3-F_2^* &= 1.744(10)\\ Al_3-F_2^* &= 1.744(10)\\ Al_3-F_1^* &= 1.802(3)\\ \hlinelabel{eq:starsec} Al_3-F_1^* &= 1.802(3)\\ \hlinelabel{es:starsec} $		Sr ₁ ²⁺ polyhedron [9]	
$\begin{split} Sr_{1}-F_{3} &= 2.422(6)\\ Sr_{1}-F_{8} &= 2.561(5)\\ Sr_{1}-F_{1} &= 2.583(4)\\ Sr_{1}-F_{1} &= 2.720(5)\\ Sr_{1}-F_{1} &= 2.72(3)\\ Sr_{1}-F_{1} &= 2.72(3)\\ Sr_{1}-F_{2} &= 2.844(3)\\ (Sr_{1}-F) &= 2.628\\ \hlinelabel{eq:stars} \\ Sr_{2}^{2,4} &\ polyhedron [9]\\ Sr_{2}-F_{4} &= 2.439(6)\\ Sr_{2}-F_{1} &= 2.484(3)\\ (Sr_{1}-F) &= 2.628\\ \hlinelabel{eq:stars} \\ Sr_{2}-F_{3} &= 2.468(6)\\ Sr_{2}-F_{7} &= 2.494(2)\\ Sr_{2}-F_{8} &= 2.565(5)\\ Sr_{2}-F_{1} &= 2.484(8)\\ Sr_{2}-F_{8} &= 2.562(5)\\ Sr_{2}-F_{8} &= 2.569(5)\\ Sr_{2}-F_{1} &= 2.582(2)\\ Sr_{2}-F_{8} &= 2.609(5)\\ Sr_{2}-F_{8} &= 2.743(9)\\ (Sr_{2}-F) &= 2.518(7)\\ F_{3}-F_{4}(-F_{11}) &= 2 \times 89.8(4)\\ F_{9}-F_{11} &= 2.5212(6)\\ Al_{1}-F_{1} &= 2 \times 1.808(6) F_{9}-Al_{1}-F_{5} &= 2 \times 90.2(4)\\ F_{9}-F_{11} &= 2.518(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 89.8(4)\\ F_{9}-F_{11} &= 2.518(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 89.8(4)\\ F_{9}-F_{11} &= 2.518(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5)\\ F_{5}-F_{11} &= 2.518(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5)\\ F_{5}-F_{11} &= 2.518(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5)\\ F_{3}-F_{11} &= 2.518(7)\\ Al_{1}-F_{5} &-Al_{2} &= 152.8(1)\\ Al_{1}-F_{1}-Al_{3} &= 153.2(3)\\ Al_{3}^{1,3} octahedron\\ Al_{2}-F_{8}^{*} &= 1.788(4)\\ Al_{2}-F_{8}^{*} &= 1.788(4)\\ Al_{2}-F_{8}^{*} &= 1.807(8)\\ Al_{2}-F_{7}^{*} &= 1.801(4)\\ Al_{2}-F_{7}^{*} &= 1.801(3)\\ Al_{3}-F_{7}^{*} &= 1.801(3)\\ Al_{3}-F_{7}^{*} &= 1.801(3)\\ Al_{3}-F_{7}^{*} &= 1.801(3)\\ Al_{3}-F_{7}^{*} &= 1.802(2)\\ \end{array}$		$Sr_1 - F_2 = 2.393(6)$	
$\begin{split} Sr_{1}-F_{9} &= 2.561(5) \\ Sr_{1}-F_{10} &= 2.583(4) \\ Sr_{1}-F_{10} &= 2.709(5) \\ Sr_{1}-F_{10} &= 2.737(5) \\ Sr_{1}-F_{1} &= 2.737(5) \\ Sr_{1}-F_{1} &= 2.737(5) \\ Sr_{1}-F_{1} &= 2.272(3) \\ Sr_{1}-F_{1} &= 2.2484(3) \\ (Sr_{1}-F) &= 2.628 \\ \hline \\ Sr_{2}^{-2}F_{13} &= 2.468(6) \\ Sr_{2}-F_{13} &= 2.468(6) \\ Sr_{2}-F_{13} &= 2.468(6) \\ Sr_{2}-F_{13} &= 2.2482(2) \\ Sr_{2}-F_{8} &= 2.2605(5) \\ Sr_{2}-F_{13} &= 2.582(2) \\ Sr_{2}-F_{1} &= 2.582(2) \\ Sr_{2}-F_{1} &= 2.582(2) \\ Sr_{2}-F_{1} &= 2.584(8) \\ Sr_{2}-F_{1} &= 2.584(8) \\ Sr_{2}-F_{1} &= 2.548(8) \\ Sr_{2}-F_{1} &= 2.5212(6) \\ Al_{1}-F_{1} &= 2 \times 1.808(6) \\ F_{9}-Al_{1}-F_{11} &= 2 \times 89.8(4) \\ F_{9}-F_{11} &= 2.531(6) \\ F_{5}-Al_{1}-F_{11} &= 2 \times 89.8(4) \\ F_{9}-F_{11} &= 2.531(6) \\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5) \\ F_{5}-F_{11} &= 2.531(6) \\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5) \\ F_{5}-F_{11} &= 2.634(7) \\ Al_{1}-F_{5} &= Al_{2} &= 152.8(1) \\ Al_{1}-F_{1}-Al_{3} &= 153.2(3) \\ \hline \\ Al_{1}^{2}-F_{13}^{*} &= 1.788(4) \\ Al_{2}-F_{13}^{*} &= 1.788(4) \\ Al_{2}-F_{13}^{*} &= 1.788(4) \\ Al_{2}-F_{13}^{*} &= 1.807(8) \\ Al_{2}-F_{5} &= 1.81(210) \\ \langle Al_{2}-F_{5} &= 1.812(10) \\ \langle Al_{2}-F_{1}^{*} &= 1.807(8) \\ Al_{2}-F_{12}^{*} &= 1.801(3) \\ Al_{3}-F_{12}^{*} &= 1.801(3) \\ Al_{3}-F_{12}^{*} &= 1.801(3) \\ Al_{3}-F_{12}^{*} &= 1.802(3) \\ \hline \\ \end{aligned}$		$Sr_1 - F_3 = 2.422(6)$	
$\begin{split} Sr_{1}-F_{1} &= 2.583(4) \\ Sr_{1}-F_{12} &= 2.681(5) \\ Sr_{1}-F_{12} &= 2.709(5) \\ Sr_{1}-F_{4} &= 2.737(5) \\ Sr_{1}-F_{4} &= 2.737(5) \\ Sr_{1}-F_{7} &= 2.844(3) \\ \langle Sr_{1}-F_{7} &= 2.844(3) \\ \langle Sr_{2}-F_{13} &= 2.449(6) \\ Sr_{2}-F_{13} &= 2.468(6) \\ Sr_{2}-F_{13} &= 2.468(6) \\ Sr_{2}-F_{13} &= 2.2482(2) \\ Sr_{2}-F_{6} &= 2.582(2) \\ Sr_{2}-F_{6} &= 2.582(2) \\ Sr_{2}-F_{6} &= 2.584(8) \\ Sr_{2}-F_{1} &= 2.618(5) \\ Sr_{2}-F_{1} &= 2.268(6) \\ Sr_{2}-F_{1} &= 2.268(6) \\ Sr_{2}-F_{1} &= 2.268(6) \\ Sr_{2}-F_{1} &= 2.568(7) \\ Sr_{2}-F_{1} &= 2.268(7) \\ Al_{1}-F_{5} &= 2 \times 1.808(6) \\ F_{9}-Al_{1}-F_{11} &= 2 \times 89.8(4) \\ F_{9}-F_{11} &= 2.531(6) \\ F_{7}-Al_{1}-F_{11} &= 2 \times 89.8(4) \\ F_{9}-F_{11} &= 2.531(6) \\ F_{7}-Al_{1}-F_{11} &= 2 \times 89.8(4) \\ F_{9}-F_{11} &= 2.531(6) \\ F_{7}-Al_{1}-F_{11} &= 2 \times 89.8(4) \\ F_{9}-F_{11} &= 2.531(6) \\ F_{7}-Al_{1}-F_{11} &= 2 \times 89.8(4) \\ F_{9}-F_{11} &= 2.531(6) \\ F_{7}-Al_{1}-F_{11} &= 2 \times 89.2(4) \\ F_{9}-F_{11} &= 2.531(6) \\ F_{7}-Al_{1}-F_{11} &= 2 \times 92.6(5) \\ F_{7}-F_{11} &= 2.531(6) \\ F_{7}-Al_{1}-F_{11} &= 2 \times 92.6(5) \\ F_{7}-F_{11} &= 2.634(7) \\ Al_{1}-F_{5} &= 1.788(4) \\ Al_{2}-F_{6}^{*} &= 1.789(4) \\ Al_{2}-F_{6}^{*} &= 1.789(4) \\ Al_{2}-F_{6}^{*} &= 1.789(4) \\ Al_{2}-F_{6}^{*} &= 1.807(8) \\ Al_{2}-F_{7}^{*} &= 1.801(4) \\ Al_{2}-F_{7}^{*} &= 1.801(4) \\ Al_{2}-F_{7}^{*} &= 1.801(4) \\ Al_{2}-F_{7}^{*} &= 1.801(3) \\ Al_{3}-F_{7}^{*} &= 1.796(2) \\ Al_{3}-F_{1}^{*} &= 1.796(2) \\ Al_{3}-F_{1}^{*} &= 1.803(3) \\ Al_{3}-F_{7}^{*} &= 1.803(3) \\ Al_{3}-F_{7}^{*} &= 1.802(3) \\ Al_{3}-F_{7}^{*$		$Sr_1 - F_8 = 2.561(5)$	
$\begin{split} Sr_{1}-F_{12} &= 2.681(5)\\ Sr_{1}-F_{10} &= 2.709(5)\\ Sr_{1}-F_{1} &= 2.737(5)\\ Sr_{1}-F_{4} &= 2.737(5)\\ Sr_{1}-F_{9} &= 2.844(3)\\ (Sr_{1}-F_{9} &= 2.844(3)\\ (Sr_{1}-F_{9} &= 2.484(3)\\ (Sr_{2}-F_{13} &= 2.488(6)\\ Sr_{2}-F_{13} &= 2.488(6)\\ Sr_{2}-F_{13} &= 2.484(2)\\ Sr_{2}-F_{8} &= 2.494(2)\\ Sr_{2}-F_{8} &= 2.565(5)\\ Sr_{2}-F_{1} &= 2.882(2)\\ Sr_{2}-F_{8} &= 2.609(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{1} &= 2.568\\ Al_{1}^{3+} \text{ octahedron}\\ Al_{1}-F_{9}^{*} &= 2 \times 1.749(4) F_{9}-Al_{1}-F_{5} &= 2 \times 90.2(4) F_{9}-F_{5} &= 2.5212(6)\\ Al_{1}-F_{3} &= 2 \times 1.808(6) F_{9}-Al_{1}-F_{1} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.540(6)\\ (Al_{1}-F_{3} &= 1.836(3) F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.540(6)\\ (Al_{1}-F_{1} &= 2 \times 1.836(3) F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.540(6)\\ (Al_{1}-F_{1} &= 1.798 F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.540(6)\\ (Al_{1}-F_{1} &= 1.798 F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.548(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5) F_{5}-F_{11} &= 2.518(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5) F_{5}-F_{11} &= 2.634(7)\\ Al_{1}-F_{3}^{*} &= 1.788(4)\\ Al_{2}-F_{3}^{*} &= 1.788(4)\\ Al_{2}-F_{3}^{*} &= 1.807(8)\\ Al_{2}-F_{3}^{*} &= 1.807(8)\\ Al_{2}-F_{3}^{*} &= 1.807(8)\\ Al_{2}-F_{3}^{*} &= 1.807(8)\\ Al_{2}-F_{3}^{*} &= 1.801(3)\\ Al_{3}-F_{4}^{*} &= 1.796(2)\\ Al_{3}-F_{4}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.802(6)\\ Al_{3}-F_{7}^{*} &= 1.802(6)\\ Al_{3}-F_{7}^{*} &= 1.802(7)\\ (Al_{3}-F_{7}^{*} &= 1.802(7)\\ (Al_{3}-F_{7$		$Sr_1 - F_1 = 2.583(4)$	
$\begin{split} Sr_{1}-F_{10} &= 2.709(5)\\ Sr_{1}-F_{1} &= 2.737(5)\\ Sr_{1}-F_{9} &= 2.844(3)\\ (Sr_{1}-F_{9} &= 2.844(3)\\ (Sr_{1}-F_{7} &= 2.844(3)\\ (Sr_{1}-F_{7} &= 2.2844(3)\\ (Sr_{2}-F_{1} &= 2.468(6)\\ Sr_{2}-F_{1} &= 2.468(6)\\ Sr_{2}-F_{7} &= 2.494(2)\\ Sr_{2}-F_{8} &= 2.565(5)\\ Sr_{2}-F_{8} &= 2.582(2)\\ Sr_{2}-F_{8} &= 2.584(8)\\ Sr_{2}-F_{8} &= 2.609(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{7} &= 2.618(5)\\ Sr_{2}-F_{7} &= 2.2688\\ Al_{1}^{3+} \text{ octahedron}\\ Al_{1}-F_{9}^{*} &= 2 \times 1.749(4) F_{9}-Al_{1}-F_{5} &= 2 \times 90.2(4) F_{9}-F_{5} &= 2.520(6)\\ Al_{1}-F_{9} &= 1.808(6) F_{9}-Al_{1}-F_{5} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.512(6)\\ Al_{1}-F_{1} &= 2 \times 1.836(3) F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.540(6)\\ (Al_{1}-F_{7} &= 1.798) F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.531(6)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5) F_{5}-F_{11} &= 2.518(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5) F_{5}-F_{11} &= 2.518(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5) F_{5}-F_{11} &= 2.634(7)\\ Al_{1}-F_{5} &= 1.788(4)\\ Al_{2}-F_{6}^{*} &= 1.788(4)\\ Al_{2}-F_{6}^{*} &= 1.788(4)\\ Al_{2}-F_{6}^{*} &= 1.788(4)\\ Al_{2}-F_{6}^{*} &= 1.789(4)\\ Al_{2}-F_{5} &= 1.801(4)\\ Al_{2}-F_{5} &= 1.801(4)\\ Al_{2}-F_{5} &= 1.801(4)\\ Al_{2}-F_{7}^{*} &= 1.801(4)\\ Al_{2}-F_{7}^{*} &= 1.801(4)\\ Al_{2}-F_{7}^{*} &= 1.801(3)\\ Al_{3}-F_{7}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.802(8)\\ Al_{3}-F_{7}^{*} &= 1.802(8)\\$		$Sr_1 - F_{12} = 2.681(5)$	
$\begin{split} Sr_{1}-F_{1} &= 2.722(3)\\ Sr_{1}-F_{4} &= 2.737(5)\\ Sr_{1}-F_{9} &= 2.844(3)\\ (Sr_{1}-F)^{-} &= 2.628\\ \\Sr_{2}^{2+} polyhedron [9]\\ Sr_{2}-F_{4} &= 2.449(6)\\ Sr_{2}-F_{13} &= 2.448(6)\\ Sr_{2}-F_{13} &= 2.468(6)\\ Sr_{2}-F_{3} &= 2.565(5)\\ Sr_{2}-F_{13} &= 2.582(2)\\ Sr_{2}-F_{6} &= 2.584(8)\\ Sr_{2}-F_{6} &= 2.584(8)\\ Sr_{2}-F_{8} &= 2.609(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{1} &= 2.618(5)\\ Sr_{2}-F_{1} &= 2.568\\ \\Al_{1}-F_{9} &= 2 \times 1.749(4) F_{9}-Al_{1}-F_{5} &= 2 \times 90.2(4) F_{9}-F_{5} &= 2.520(6)\\ Al_{1}-F_{9} &= 2 \times 1.808(6) F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.540(6)\\ (Al_{1}-F_{9} &= 1.798 F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4) F_{9}-F_{11} &= 2.540(6)\\ (Al_{1}-F) &= 1.798 F_{9}-Al_{1}-F_{11} &= 2 \times 89.8(4) F_{9}-F_{11} &= 2.511(6)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 89.8(4) F_{9}-F_{11} &= 2.518(7)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5) F_{5}-F_{11} &= 2.634(7)\\ Al_{1}-F_{5} -Al_{2} &= 152.8(1)\\ Al_{2}-F_{10}^{*} &= 1.788(4)\\ Al_{2}-F_{10}^{*} &= 1.788(4)\\ Al_{2}-F_{10}^{*} &= 1.788(4)\\ Al_{2}-F_{10}^{*} &= 1.789(4)\\ Al_{2}-F_{10}^{*} &= 1.801(4)\\ Al_{2}-F_{8}^{*} &= 1.807(8)\\ Al_{3}-F_{2}^{*} &= 1.807(8)\\ Al_{3}-F_{2}^{*} &= 1.744(10)\\ Al_{3}-F_{2}^{*} &= 1.796(2)\\ Al_{3}-F_{12}^{*} &= 1.808(8)\\ Al_{3}-F_{1}^{*} &= 1.802(6)\\ \end{array}$		$Sr_1 - F_{10} = 2.709(5)$	
$\begin{split} Sr_{1}-F_{4} &= 2.737(5)\\ Sr_{1}-F_{9} &= 2.844(3)\\ \langle Sr_{1}-F\rangle &= 2.628\\ Sr_{2}^{2+} polyhedron [9]\\ Sr_{2}-F_{4} &= 2.449(6)\\ Sr_{2}-F_{13} &= 2.468(6)\\ Sr_{2}-F_{7} &= 2.494(2)\\ Sr_{2}-F_{8} &= 2.565(5)\\ Sr_{2}-F_{8} &= 2.584(8)\\ Sr_{2}-F_{8} &= 2.584(8)\\ Sr_{2}-F_{8} &= 2.584(8)\\ Sr_{2}-F_{8} &= 2.609(5)\\ Sr_{2}-F_{1} &= 2.584(8)\\ Sr_{2}-F_{3} &= 2.743(9)\\ \langle Sr_{2}-F_{3} &= 2.743(9)\\ \langle Sr_{2}-F_{3} &= 2.743(9)\\ \langle Sr_{2}-F_{3} &= 2.743(9)\\ \langle Sr_{2}-F_{3} &= 2.884(8)\\ F_{9}-F_{1} &= 2.884(8)\\ Al_{1}-F_{9} &= 2 \times 1.808(6)\\ F_{9}-Al_{1}-F_{5} &= 2 \times 90.2(4)\\ F_{9}-F_{1} &= 2.520(6)\\ Al_{1}-F_{3} &= 2 \times 1.808(6)\\ F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4)\\ F_{9}-F_{11} &= 2.540(6)\\ \langle Al_{1}-F\rangle &= 1.798\\ F_{9}-Al_{1}-F_{11} &= 2 \times 89.8(4)\\ F_{9}-F_{11} &= 2.531(6)\\ F_{5}-Al_{1}-F_{11} &= 2 \times 89.8(4)\\ Al_{2}-F_{1} &= 1.52.8(1)\\ Al_{1}-F_{1}-F_{11} &= 1.53.2(3)\\ \hline Al_{1}^{3+} octahedron\\ Al_{2}-F_{13}^{*} &= 1.788(4)\\ Al_{2}-F_{6}^{*} &= 1.801(4)\\ Al_{2}-F_{6}^{*} &= 1.801(4)\\ Al_{2}-F_{6}^{*} &= 1.807(8)\\ Al_{2}-F_{5} &= 1.812(10)\\ \langle Al_{2}-F_{1} &= 1.796(2)\\ Al_{3}-F_{2}^{*} &= 1.796(2)\\ Al_{3}-F_{12}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.808(8)\\ Al_{3}-F_{7}^{*} &= 1.802(6)\\ \hline Al$		$Sr_1 - F_1 = 2.722(3)$	
$\begin{split} Sr_1-F_9 &= 2.844(3)\\ \langle Sr_1-F\rangle &= 2.628\\ Sr_2^{2^+} polyhedron [9]\\ Sr_2-F_4 &= 2.449(6)\\ Sr_2-F_3 &= 2.494(2)\\ Sr_2-F_7 &= 2.494(2)\\ Sr_2-F_7 &= 2.494(2)\\ Sr_2-F_7 &= 2.494(2)\\ Sr_2-F_7 &= 2.582(2)\\ Sr_2-F_7 &= 2.582(2)\\ Sr_2-F_8 &= 2.609(5)\\ Sr_2-F_8 &= 2.609(5)\\ Sr_2-F_7 &= 2.618(5)\\ Sr_2-F_7 &= 2.618(5)\\ Sr_2-F_7 &= 2.618(5)\\ Sr_2-F_7 &= 2.618(5)\\ Sr_2-F_7 &= 2.568\\ Al_1^{+^+} octahedron\\ Al_1-F_5 &= 2 \times 1.808(6) F_9-Al_1-F_5 &= 2 \times 89.8(4)\\ F_9-F_1 &= 2.531(6)\\ \langle Al_1-F_7 &= 1.798 F_9-Al_1-F_{11} &= 2 \times 89.8(4)\\ F_9-F_{11} &= 2 \times 87.4(5) F_5-F_{11} &= 2.531(6)\\ \langle Al_1-F_7 &= 1.798 F_9-Al_1-F_{11} &= 2 \times 87.4(5) F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 87.4(5) F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_3-F_{11} &= 2.634(7)\\ Al_1-F_5 &= 1.788(4)\\ Al_2-F_6^* &= 1.788(4)\\ Al_2-F_6^* &= 1.788(4)\\ Al_2-F_6^* &= 1.788(4)\\ Al_2-F_6^* &= 1.801(4)\\ Al_2-F_8^* &= 1.807(8)\\ Al_2-F_7 &= 1.812(10)\\ \langle Al_2-F_7 &= 1.812(10)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(7)\\ \langle Al_3-F_1 &= 1.838(7)\\ \langle Al_3-F_1 &= 1.838(7)\\ \langle Al_3-F_1 &= 1.802\\ \end{split}$		$Sr_1 - F_4 = 2.737(5)$	
$ \langle Sr_1 - F \rangle = 2.628 \\ Sr_2^{2+} polyhedron [9] \\ Sr_2 - F_4 = 2.449(6) \\ Sr_2 - F_1_3 = 2.468(6) \\ Sr_2 - F_1_3 = 2.582(2) \\ Sr_2 - F_8 = 2.669(5) \\ Sr_2 - F_1 = 2.582(2) \\ Sr_2 - F_6 = 2.584(8) \\ Sr_2 - F_1 = 2.618(5) \\ Sr_2 - F_1 = 2.618(5) \\ Sr_2 - F_1 = 2.618(5) \\ Sr_2 - F_2 = 2.568 \\ Al_1^{3+} \text{ octahedron} \\ Al_1 - F_9^* = 2 \times 1.808(6) F_9 - Al_1 - F_5 = 2 \times 89.8(4) \\ F_9 - F_5 = 2.512(6) \\ Al_1 - F_1 = 2 \times 1.808(6) F_9 - Al_1 - F_{11} = 2 \times 90.2(4) \\ F_9 - F_1 = 2.531(6) \\ F_9 - Al_1 - F_{11} = 2 \times 89.8(4) \\ F_9 - F_{11} = 2.531(6) \\ F_7 - Al_1 - F_{11} = 2 \times 89.8(4) \\ F_9 - F_{11} = 2.531(6) \\ F_7 - Al_1 - F_{11} = 2 \times 89.8(4) \\ F_9 - F_{11} = 2.518(7) \\ F_5 - Al_1 - F_{11} = 2 \times 92.6(5) \\ F_5 - Al_1 - F_{11} = 2 \times 92.6(5) \\ F_5 - Al_1 - F_{11} = 2 \times 92.6(5) \\ F_9 - F_{11} = 2.634(7) \\ Al_1 - F_5 - Al_2 = 152.8(1) \\ Al_2 - F_6^* = 1.789(4) \\ Al_2 - F_6^* = 1.789(4) \\ Al_2 - F_8^* = 1.801(4) \\ Al_2 - F_8^* = 1.801(4) \\ Al_2 - F_8 = 1.801(4) \\ Al_2 - F_8 = 1.801(4) \\ Al_2 - F_8 = 1.801(4) \\ Al_3 - F_7^* = 1.801(3) \\ Al_3 - F_1^* = 1.801(3) \\ Al_3 - F_1^* = 1.808(8) \\ Al_3 - F_1^* = 1.802(6) \\ Al_3 - F_1 = 1.838(7) \\ \langle Al_3 - F_1 = 1.838(7) \\ \langle Al_3 - F_1 = 1.802(6) \\ Al_3 - F_$		$Sr_1 - F_9 = 2.844(3)$	
$\begin{split} Sr_2^{2^+} & \text{polyhedron [9]} \\ Sr_2-F_4 &= 2.449(6) \\ Sr_2-F_1_3 &= 2.468(6) \\ Sr_2-F_1_3 &= 2.582(2) \\ Sr_2-F_8 &= 2.565(5) \\ Sr_2-F_1 &= 2.582(2) \\ Sr_2-F_6 &= 2.584(8) \\ Sr_2-F_8 &= 2.609(5) \\ Sr_2-F_1 &= 2.618(5) \\ Sr_2-F_1 &= 2.618(5) \\ Sr_2-F_1 &= 2.618(5) \\ Sr_2-F_1 &= 2.568 \\ \hline Al_1^{1^+} & \text{octahedron} \\ Al_1-F_3 &= 2 \times 1.749(4) F_9-Al_1-F_5 &= 2 \times 89.8(4) F_9-F_5 &= 2.520(6) \\ Al_1-F_3 &= 2 \times 1.836(3) F_9-Al_1-F_{11} &= 2 \times 90.2(4) F_9-F_{11} &= 2.540(6) \\ (Al_1-F_1 &= 2 \times 1.836(3) F_9-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.540(6) \\ (Al_1-F_1 &= 2 \times 1.836(3) F_9-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.518(7) \\ F_5-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.518(7) \\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_5-F_{11} &= 2.634(7) \\ Al_1-F_5 &-Al_2 &= 152.8(1) \\ Al_2-F_6^* &= 1.789(4) \\ Al_2-F_6^* &= 1.789(4) \\ Al_2-F_6^* &= 1.789(4) \\ Al_2-F_8^* &= 1.801(4) \\ Al_2-F_8^* &= 1.801(4) \\ Al_2-F_6^* &= 1.796(4) \\ Al_2-F_6 &= 1.799 \\ \hline Al_3^{1^+} & \text{octahedron} \\ Al_3-F_1^* &= 1.801(3) \\ Al_3-F_1^* &= 1.801(3) \\ Al_3-F_1^* &= 1.801(3) \\ Al_3-F_1^* &= 1.802(6) \\ \hline Al_3-F_1 &= 1.838(7) \\ (Al_3-F_1) &= 1.802 \\ \hline \end{split}$		$\langle Sr_1 - F \rangle = 2.628$	
$\begin{split} Sr_2-F_4 &= 2.449(6)\\ Sr_2-F_{13} &= 2.468(6)\\ Sr_2-F_{13} &= 2.468(6)\\ Sr_2-F_1 &= 2.585(2)\\ Sr_2-F_1 &= 2.582(2)\\ Sr_2-F_1 &= 2.582(2)\\ Sr_2-F_1 &= 2.609(5)\\ Sr_2-F_1 &= 2.618(5)\\ Sr_2-F_3 &= 2.743(9)\\ (Sr_2-F) &= 2.568\\ \hline Al_1^{3^+} \ octahedron\\ Al_1-F_9 &= 2 \times 1.808(6) \ F_9-Al_1-F_5 &= 2 \times 90.2(4) \ F_9-F_5 &= 2.520(6)\\ Al_1-F_5 &= 2 \times 1.808(6) \ F_9-Al_1-F_5 &= 2 \times 90.2(4) \ F_9-F_1 &= 2.540(6)\\ (Al_1-F) &= 1.798 \ F_9-Al_1-F_{11} &= 2 \times 90.2(4) \ F_9-F_{11} &= 2.540(6)\\ (Al_1-F) &= 1.798 \ F_9-Al_1-F_{11} &= 2 \times 92.6(5) \ F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) \ F_5-F_{11} &= 2.634(7)\\ Al_2-F_6 &= 1.788(4) \\ Al_2-F_6 &= 1.789(4) \\ Al_2-F_8 &= 1.801(4) \\ Al_2-F_8 &= 1.801(4) \\ Al_2-F_8 &= 1.801(4) \\ Al_2-F_8 &= 1.801(2) \\ Al_3-F_4 &= 1.796(2) \\ Al_3-F_1 &= 1.822(6) \\ Al_3-F_1 &= 1.801(2) \\ Al_3-F_1 &= 1.802(2) \\ \end{split}$		Sr ₂ ²⁺ polyhedron [9]	
$\begin{split} Sr_2-F_{13} &= 2.468(6)\\ Sr_2-F_7 &= 2.494(2)\\ Sr_2-F_8 &= 2.565(5)\\ Sr_2-F_{13} &= 2.582(2)\\ Sr_2-F_8 &= 2.584(8)\\ Sr_2-F_8 &= 2.609(5)\\ Sr_2-F_8 &= 2.609(5)\\ Sr_2-F_1 &= 2.618(5)\\ Sr_2-F_3 &= 2.743(9)\\ (\langle Sr_2-F\rangle &= 2.568\\ & Al_1^{3+} \ octahedron\\ Al_1-F_9 &= 2 \times 1.808(6) \ F_9-Al_1-F_5 &= 2 \times 90.2(4) \qquad F_9-F_5 &= 2.520(6)\\ Al_1-F_5 &= 2 \times 1.808(6) \ F_9-Al_1-F_5 &= 2 \times 90.2(4) \qquad F_9-F_{11} &= 2.531(6)\\ (Al_1-F_1 &= 2 \times 1.836(3) \ F_9-Al_1-F_{11} &= 2 \times 89.8(4) \qquad F_9-F_{11} &= 2.531(6)\\ (Al_1-F) &= 1.798 \qquad F_9-Al_1-F_{11} &= 2 \times 87.4(5) \qquad F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) \qquad F_5-F_{11} &= 2.634(7)\\ Al_1-F_5 -Al_2 &= 152.8(1)\\ Al_2-F_6^* &= 1.798(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.807(8)\\ Al_2-F_7 &= 1.812(10)\\ (\langle Al_2-F\rangle &= 1.799 \qquad Al_3^{3+} \ octahedron\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.802(6)\\ Al_3-F_1^* &= 1.802(6) \\ Al_3-F_1^* &= 1.80(6) \\ Al_3-F_1^* &= 1.80(6) \\ Al_3-F_1^* &= 1.80(6) \\ A$		$Sr_2 - F_4 = 2.449(6)$	
$\begin{split} Sr_2-F_7 &= 2.494(2)\\ Sr_2-F_8 &= 2.565(5)\\ Sr_2-F_{11} &= 2.582(2)\\ Sr_2-F_6 &= 2.584(8)\\ Sr_2-F_8 &= 2.609(5)\\ Sr_2-F_1 &= 2.618(5)\\ Sr_2-F_3 &= 2.743(9)\\ \langle Sr_2-F \rangle &= 2.568\\ \hline Al_1^{3^+} \ octahedron\\ Al_1-F_5 &= 2 \times 1.808(6) \ F_9-Al_1-F_5 &= 2 \times 90.2(4) F_9-F_5 &= 2.520(6)\\ Al_1-F_5 &= 2 \times 1.808(6) \ F_9-Al_1-F_5 &= 2 \times 89.8(4) F_9-F_1 &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 1.836(3) \ F_9-Al_1-F_{11} &= 2 \times 90.2(4) F_9-F_{11} &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 1.836(3) \ F_9-Al_1-F_{11} &= 2 \times 90.2(4) F_9-F_{11} &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 1.836(3) \ F_9-Al_1-F_{11} &= 2 \times 90.2(4) F_9-F_{11} &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 1.836(3) \ F_9-Al_1-F_{11} &= 2 \times 90.2(4) F_9-F_{11} &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 1.836(3) \ F_9-Al_1-F_{11} &= 2 \times 90.2(4) F_9-F_{11} &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 92.6(5) F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_5-F_{11} &= 2.634(7)\\ Al_1-F_5 &= Al_2 &= 152.8(1)\\ Al_1-F_1 &= Al_2 &= 152.8(1)\\ Al_2-F_1^* &= 1.788(4)\\ Al_2-F_6^* &= 1.789(4)\\ Al_2-F_6^* &= 1.789(4)\\ Al_2-F_6^* &= 1.789(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.801(3)\\ Al_3-F_1^* &= 1.801(3)\\ Al_3-F_1^* &= 1.801(3)\\ Al_3-F_1^* &= 1.801(3)\\ Al_3-F_1^* &= 1.802(6)\\ Al_3-F_1^* &= 1.80(6)\\ Al_$		$Sr_2 - F_{13} = 2.468(6)$	
$\begin{split} Sr_2-F_8 &= 2.565(5)\\ Sr_2-F_{13} &= 2.582(2)\\ Sr_2-F_6 &= 2.584(8)\\ Sr_2-F_8 &= 2.609(5)\\ Sr_2-F_1 &= 2.618(5)\\ Sr_2-F_1 &= 2.618(5)\\ Sr_2-F_3 &= 2.743(9)\\ \langle Sr_2-F \rangle &= 2.568\\ &Al_1^{3+} \text{ octahedron}\\ Al_1-F_5 &= 2 \times 1.749(4) F_9-Al_1-F_5 &= 2 \times 90.2(4) F_9-F_5 &= 2.512(6)\\ Al_1-F_5 &= 2 \times 1.808(6) F_9-Al_1-F_1 &= 2 \times 90.2(4) F_9-F_{11} &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 1.836(3) F_9-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 1.836(3) F_9-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 1.836(3) F_9-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.540(6)\\ \langle Al_1-F_1 &= 2 \times 1.836(3) F_9-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_5-F_{11} &= 2.634(7)\\ Al_1-F_5-Al_2 &= 152.8(1)\\ Al_2-F_6 &= 1.789(4)\\ Al_2-F_6 &= 1.789(4)\\ Al_2-F_6 &= 1.789(4)\\ Al_2-F_6 &= 1.789(4)\\ Al_2-F_8 &= 1.801(4)\\ Al_2-F_8 &= 1.807(8)\\ Al_2-F_7 &= 1.801(3)\\ Al_3-F_4 &= 1.796(2)\\ Al_3-F_1 &= 1.822(6)\\ Al_3-F_1 &= 1.838(7)\\ \langle Al_3-F_1 &= 1.838(7)\\ \langle Al_3-F_1 &= 1.802\\ \end{split}$		$Sr_2 - F_7 = 2.494(2)$	
$\begin{split} Sr_2-F_{13} &= 2.582(2)\\ Sr_2-F_6 &= 2.584(8)\\ Sr_2-F_8 &= 2.609(5)\\ Sr_2-F_1 &= 2.618(5)\\ Sr_2-F_3 &= 2.743(9)\\ \langle Sr_2-F \rangle &= 2.568\\ \hline Al_1^{1+} \text{ octahedron}\\ Al_1-F_5 &= 2 \times 1.749(4) F_9-Al_1-F_5 &= 2 \times 90.2(4) F_9-F_5 &= 2.520(6)\\ Al_1-F_5 &= 2 \times 1.808(6) F_9-Al_1-F_5 &= 2 \times 89.8(4) F_9-F_{11} &= 2.512(6)\\ Al_1-F_1 &= 2 \times 1.836(3) F_9-Al_1-F_{11} &= 2 \times 90.2(4) F_9-F_{11} &= 2.531(6)\\ (Al_1-F) &= 1.798 F_9-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_5-F_{11} &= 2.634(7)\\ Al_1-F_5 &-Al_2 &= 152.8(1)\\ Al_2-F_6^* &= 1.788(4)\\ Al_2-F_6^* &= 1.788(4)\\ Al_2-F_6^* &= 1.789(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_5 &= 1.812(10)\\ \langle Al_2-F \rangle &= 1.799\\ \hline Al_3^{3+} \text{ octahedron}\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(7)\\ Al_3-F_1^* &= 1.808(7)\\ Al_3-F_1^* &= 1.808(7)\\ Al_3-F_1^* &= 1.808(7)\\ \langle Al_3-F_1 &= 1.808(7$		$Sr_2 - F_8 = 2.565(5)$	
$\begin{split} Sr_2-F_6 &= 2.584(8)\\ Sr_2-F_8 &= 2.609(5)\\ Sr_2-F_1 &= 2.618(5)\\ Sr_2-F_3 &= 2.743(9)\\ \langle Sr_2-F \rangle &= 2.568\\ \hline Al_1^{++} \text{ octahedron}\\ Al_1-F_9 &= 2 \times 1.749(4) F_9-Al_1-F_5 &= 2 \times 90.2(4) F_9-F_5 &= 2.520(6)\\ Al_1-F_5 &= 2 \times 1.808(6) F_9-Al_1-F_5 &= 2 \times 89.8(4) F_9-F_5 &= 2.512(6)\\ Al_1-F_1 &= 2 \times 1.836(3) F_9-Al_1-F_{11} &= 2 \times 90.2(4) F_9-F_{11} &= 2.518(6)\\ \langle Al_1-F \rangle &= 1.798 F_9-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_5-F_{11} &= 2.634(7)\\ Al_1-F_5 &-Al_2 &= 152.8(1)\\ Al_2-F_6^* &= 1.788(4)\\ Al_2-F_6^* &= 1.788(4)\\ Al_2-F_6^* &= 1.789(4)\\ Al_2-F_6^* &= 1.789(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.807(8)\\ Al_2-F_7 &= 1.812(10)\\ \langle Al_2-F \rangle &= 1.799\\ \hline Al_3^{3+} \text{ octahedron}\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(7)\\ \langle Al_3-F_1 &= 1.838(7)\\ \langle Al_3-F_1 &= 1.838(7)\\ \langle Al_3-F_1 &= 1.802\\ \end{split}$		$Sr_2 - F_{13} = 2.582(2)$	
$\begin{split} Sr_2-F_8 &= 2.609(5)\\ Sr_2-F_1 &= 2.618(5)\\ Sr_2-F_3 &= 2.743(9)\\ (Sr_2-F) &= 2.568\\ \\ Al_1^{3^+} \ octahedron\\ Al_1-F_9 &= 2 \times 1.749(4) \ F_9-Al_1-F_5 &= 2 \times 90.2(4) \ F_9-F_5 &= 2.520(6)\\ Al_1-F_5 &= 2 \times 1.808(6) \ F_9-Al_1-F_5 &= 2 \times 89.8(4) \ F_9-F_5 &= 2.512(6)\\ Al_1-F_{11} &= 2 \times 1.836(3) \ F_9-Al_1-F_{11} &= 2 \times 90.2(4) \ F_9-F_{11} &= 2.540(6)\\ (Al_1-F) &= 1.798 \ F_9-Al_1-F_{11} &= 2 \times 89.8(4) \ F_9-F_{11} &= 2.531(6)\\ F_5-Al_1-F_{11} &= 2 \times 87.4(5) \ F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) \ F_5-F_{11} &= 2.634(7)\\ Al_1-F_5 &-Al_2 &= 152.8(1)\\ Al_1-F_5 -Al_2 &= 153.2(3)\\ \\ Al_2^{3^+} \ octahedron\\ Al_2-F_{13}^* &= 1.788(4)\\ Al_2-F_6^* &= 1.789(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.801(4)\\ Al_2-F_8^* &= 1.812(10)\\ (Al_2-F) &= 1.799\\ \\ \\ Al_3^{3^+} \ octahedron\\ Al_3-F_2^* &= 1.744(10)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(7)\\ (Al_3-F) &= 1.802\\ \\ \end{split}$		$Sr_2 - F_6 = 2.584(8)$	
$\begin{split} Sr_2-F_1 &= 2.618(5)\\ Sr_2-F_3 &= 2.743(9)\\ (Sr_2-F) &= 2.568\\ &Al_1^{3^+} \mbox{ octahedron}\\ Al_1-F_9 &= 2 \times 1.749(4) \ F_9-Al_1-F_5 &= 2 \times 90.2(4) \ F_9-F_5 &= 2.520(6)\\ Al_1-F_5 &= 2 \times 1.808(6) \ F_9-Al_1-F_5 &= 2 \times 89.8(4) \ F_9-F_5 &= 2.512(6)\\ Al_1-F_{11} &= 2 \times 1.836(3) \ F_9-Al_1-F_{11} &= 2 \times 90.2(4) \ F_9-F_{11} &= 2.540(6)\\ (Al_1-F) &= 1.798 \ F_9-Al_1-F_{11} &= 2 \times 89.8(4) \ F_9-F_{11} &= 2.531(6)\\ F_5-Al_1-F_{11} &= 2 \times 87.4(5) \ F_5-F_{11} &= 2.518(7)\\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) \ F_5-F_{11} &= 2.518(7)\\ Al_1-F_5 &-Al_2 &= 152.8(1)\\ Al_1-F_5 &-Al_2 &= 152.8(1)\\ Al_1-F_5 &-Al_2 &= 153.2(3)\\ \hline Al_2^{3^+} \ octahedron\\ Al_2-F_{13}^* &= 1.788(4)\\ Al_2-F_6^* &= 1.789(4)\\ Al_2-F_6^* &= 1.799(4)\\ Al_2-F_8^* &= 1.807(8)\\ Al_2-F_5 &= 1.812(10)\\ (Al_2-F) &= 1.799\\ \hline Al_3^{3^+} \ octahedron\\ Al_3-F_2^* &= 1.744(10)\\ Al_3-F_4^* &= 1.796(2)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.808(8)\\ Al_3-F_1^* &= 1.838(7)\\ (Al_3-F) &= 1.802\\ \end{split}$		$Sr_2 - F_8 = 2.609(5)$	
$\begin{split} Sr_2-F_3 &= 2.743(9) \\ \langle Sr_2-F \rangle &= 2.568 \\ & Al_1^{3^+} \text{ octahedron} \\ Al_1-F_9^* &= 2 \times 1.749(4) \ F_9-Al_1-F_5 &= 2 \times 90.2(4) F_9-F_5 &= 2.520(6) \\ Al_1-F_5 &= 2 \times 1.808(6) \ F_9-Al_1-F_5 &= 2 \times 89.8(4) F_9-F_5 &= 2.512(6) \\ Al_1-F_1 &= 2 \times 1.836(3) \ F_9-Al_1-F_{11} &= 2 \times 90.2(4) F_9-F_{11} &= 2.540(6) \\ \langle Al_1-F \rangle &= 1.798 F_9-Al_1-F_{11} &= 2 \times 89.8(4) F_9-F_{11} &= 2.531(6) \\ F_5-Al_1-F_{11} &= 2 \times 87.4(5) F_5-F_{11} &= 2.518(7) \\ F_5-Al_1-F_{11} &= 2 \times 92.6(5) F_5-F_{11} &= 2.634(7) \\ Al_1-F_5 &-Al_2 &= 152.8(1) \\ Al_1-F_{11}-Al_3 &= 153.2(3) \\ & Al_2^{3^+} \text{ octahedron} \\ Al_2-F_{13}^* &= 1.788(4) \\ Al_2-F_0^* &= 1.789(4) \\ Al_2-F_0^* &= 1.796(4) \\ Al_2-F_5 &= 1.812(10) \\ \langle Al_2-F \rangle &= 1.799 \\ & Al_3^{3^+} \text{ octahedron} \\ Al_3-F_2^* &= 1.744(10) \\ Al_3-F_1^* &= 1.808(8) \\ Al_3-F_1^* &= 1.802(6) \\ Al_3-F \rangle &= 1.802 \\ \end{split}$		$Sr_2 - F_1 = 2.618(5)$	
$ \langle Sr_2 - F \rangle = 2.368 $ $ Al_1^{3^+} \text{ octahedron} $ $ Al_1 - F_9^* = 2 \times 1.749(4) F_9 - Al_1 - F_5 = 2 \times 90.2(4) F_9 - F_5 = 2.520(6) $ $ Al_1 - F_5 = 2 \times 1.808(6) F_9 - Al_1 - F_5 = 2 \times 89.8(4) F_9 - F_5 = 2.512(6) $ $ Al_1 - F_{11} = 2 \times 1.836(3) F_9 - Al_1 - F_{11} = 2 \times 90.2(4) F_9 - F_{11} = 2.540(6) $ $ \langle Al_1 - F \rangle = 1.798 F_9 - Al_1 - F_{11} = 2 \times 89.8(4) F_9 - F_{11} = 2.531(6) $ $ F_5 - Al_1 - F_{11} = 2 \times 87.4(5) F_5 - F_{11} = 2.518(7) $ $ F_5 - Al_1 - F_{11} = 2 \times 92.6(5) F_5 - F_{11} = 2.518(7) $ $ Al_1 - F_5 - Al_2 = 152.8(1) $ $ Al_2 - F_{13}^* = 1.788(4) $ $ Al_2 - F_6^* = 1.796(4) $ $ Al_2 - F_5^* = 1.801(4) $ $ Al_2 - F_5 = 1.812(10) $ $ \langle Al_2 - F \rangle = 1.799 $ $ Al_3^{3^+} \text{ octahedron} $ $ Al_3 - F_2^* = 1.744(10) $ $ Al_3 - F_1^* = 1.808(8) $ $ Al_3 - F_1^* = 1.838(7) $ $ \langle Al_3 - F \rangle = 1.802 $		$Sr_2 - F_3 = 2.743(9)$	
$Al_{1}^{3+} \text{ octahedron}$ $Al_{1}-F_{9}^{*} = 2 \times 1.749(4) F_{9}-Al_{1}-F_{5} = 2 \times 90.2(4) F_{9}-F_{5} = 2.520(6)$ $Al_{1}-F_{5} = 2 \times 1.808(6) F_{9}-Al_{1}-F_{5} = 2 \times 89.8(4) F_{9}-F_{5} = 2.512(6)$ $Al_{1}-F_{11} = 2 \times 1.836(3) F_{9}-Al_{1}-F_{11} = 2 \times 90.2(4) F_{9}-F_{11} = 2.540(6)$ $(Al_{1}-F) = 1.798 F_{9}-Al_{1}-F_{11} = 2 \times 89.8(4) F_{9}-F_{11} = 2.531(6)$ $F_{5}-Al_{1}-F_{11} = 2 \times 87.4(5) F_{5}-F_{11} = 2.518(7)$ $F_{5}-Al_{1}-F_{11} = 2 \times 92.6(5) F_{5}-F_{11} = 2.634(7)$ $Al_{1}-F_{5}-Al_{2} = 152.8(1)$ $Al_{2}-F_{13}^{*} = 1.788(4)$ $Al_{2}-F_{13}^{*} = 1.788(4)$ $Al_{2}-F_{13}^{*} = 1.788(4)$ $Al_{2}-F_{13}^{*} = 1.789(4)$ $Al_{2}-F_{3}^{*} = 1.801(4)$ $Al_{2}-F_{8}^{*} = 1.807(8)$ $Al_{2}-F_{5} = 1.812(10)$ $\langle Al_{2}-F\rangle = 1.799$ $Al_{3}^{3+} \text{ octahedron}$ $Al_{3}-F_{2}^{*} = 1.744(10)$ $Al_{3}-F_{4}^{*} = 1.796(2)$ $Al_{3}-F_{12}^{*} = 1.801(3)$ $Al_{3}-F_{1}^{*} = 1.808(8)$ $Al_{3}-F_{1}^{*} = 1.802(6)$		$\langle Sr_2 - F \rangle = 2.568$	
$\begin{array}{rcl} Al_{l}-F_{9}^{*} &= 2 \times 1.749(4) \ F_{9}-Al_{l}-F_{5} &= 2 \times 90.2(4) & F_{9}-F_{5} &= 2.520(6) \\ Al_{l}-F_{5} &= 2 \times 1.808(6) \ F_{9}-Al_{l}-F_{5} &= 2 \times 89.8(4) & F_{9}-F_{5} &= 2.512(6) \\ Al_{l}-F_{11} &= 2 \times 1.836(3) \ F_{9}-Al_{l}-F_{11} &= 2 \times 90.2(4) & F_{9}-F_{11} &= 2.540(6) \\ (Al_{l}-F) &= & 1.798 & F_{9}-Al_{l}-F_{11} &= 2 \times 89.8(4) & F_{9}-F_{11} &= 2.531(6) \\ & F_{5}-Al_{l}-F_{11} &= 2 \times 87.4(5) & F_{5}-F_{11} &= 2.518(7) \\ & F_{5}-Al_{l}-F_{11} &= 2 \times 92.6(5) & F_{5}-F_{11} &= 2.518(7) \\ & Al_{l}-F_{5}-Al_{2} &= & 152.8(1) \\ & Al_{l}-F_{5}-Al_{2} &= & 152.8(1) \\ & Al_{2}-F_{13}^{*} &= 1.788(4) \\ & Al_{2}-F_{6}^{*} &= 1.789(4) \\ & Al_{2}-F_{6}^{*} &= 1.789(4) \\ & Al_{2}-F_{8}^{*} &= 1.801(4) \\ & Al_{2}-F_{5} &= 1.812(10) \\ & \langle Al_{2}-F \rangle &= 1.799 \\ \hline & Al_{3}^{3+} \text{ octahedron} \\ & Al_{3}-F_{2}^{*} &= 1.801(3) \\ & Al_{3}-F_{12}^{*} &= 1.801(3) \\ & Al_{3}-F_{12}^{*} &= 1.808(8) \\ & Al_{3}-F_{1}^{*} &= 1.808(8) \\ & Al_{3}-F_{1}^{*} &= 1.802(6) \\ \hline & Al_{3}-F_{1}$		Al ³⁺ octahedron	
$\begin{array}{rcl} Al_{1}-F_{5} &= 2 \times 1.808(6) \ F_{9}-Al_{1}-F_{5} &= 2 \times 89.8(4) & F_{9}-F_{5} &= 2.512(6) \\ Al_{1}-F_{11} &= 2 \times 1.836(3) \ F_{9}-Al_{1}-F_{11} &= 2 \times 90.2(4) & F_{9}-F_{11} &= 2.540(6) \\ (Al_{1}-F) &= & 1.798 & F_{9}-Al_{1}-F_{11} &= 2 \times 89.8(4) & F_{9}-F_{11} &= 2.531(6) \\ & F_{5}-Al_{1}-F_{11} &= 2 \times 87.4(5) & F_{5}-F_{11} &= 2.518(7) \\ & F_{5}-Al_{1}-F_{11} &= 2 \times 92.6(5) & F_{5}-F_{11} &= 2.518(7) \\ & Al_{1}-F_{5}-Al_{2} &= & 152.8(1) \\ & Al_{1}-F_{5}-Al_{2} &= & 152.8(1) \\ & Al_{2}-F_{13}^{*} &= 1.788(4) \\ & Al_{2}-F_{6}^{*} &= 1.789(4) \\ & Al_{2}-F_{6}^{*} &= 1.789(4) \\ & Al_{2}-F_{6}^{*} &= 1.801(4) \\ & Al_{2}-F_{5} &= 1.812(10) \\ & \langle Al_{2}-F \rangle &= 1.799 \\ \hline & Al_{3}^{3+} \text{ octahedron} \\ & Al_{3}-F_{2}^{*} &= 1.801(3) \\ & Al_{3}-F_{12}^{*} &= 1.801(3) \\ & Al_{3}-F_{12}^{*} &= 1.808(8) \\ & Al_{3}-F_{1}^{*} &= 1.802(6) \\ \hline & Al_{3}-F_{1}^{*} &= 1.802 \\ \hline \end{array}$	$Al_{1}-F_{9}^{*} = 2 \times 1.749(4)$ F	$F_9 - Al_1 - F_5 = 2 \times 90.2(4)$	$F_{9}-F_{5} = 2.520(6)$
$\begin{array}{rcl} Al_1-F_{11}&=2\times 1.836(3) \ F_{9}-Al_{1}-F_{11}&=2\times 90.2(4) & F_{9}-F_{11}&=2.540(6) \\ (Al_{1}-F)&=& 1.798 & F_{9}-Al_{1}-F_{11}&=2\times 89.8(4) & F_{9}-F_{11}&=2.531(6) \\ & F_{5}-Al_{1}-F_{11}&=2\times 87.4(5) & F_{5}-F_{11}&=2.518(7) \\ & F_{5}-Al_{1}-F_{11}&=2\times 92.6(5) & F_{5}-F_{11}&=2.634(7) \\ & Al_{1}-F_{5}-Al_{2}&=& 152.8(1) \\ & Al_{1}-F_{11}-Al_{3}&=& 153.2(3) \\ & & Al_{2}^{3+} \ octahedron \\ & Al_{2}-F_{6}^{*}&=1.788(4) \\ & Al_{2}-F_{6}^{*}&=1.789(4) \\ & Al_{2}-F_{6}^{*}&=1.801(4) \\ & Al_{2}-F_{8}^{*}&=1.807(8) \\ & Al_{2}-F_{5}&=&1.812(10) \\ & \langle Al_{2}-F\rangle&=&1.799 \\ & & Al_{3}^{3+} \ octahedron \\ & Al_{3}-F_{2}^{*}&=1.801(3) \\ & Al_{3}-F_{1}^{*}&=&1.808(8) \\ & Al_{3}-F_{1}^{*}&=&1.808(8) \\ & Al_{3}-F_{1}^{*}&=&1.838(7) \\ & \langle Al_{3}-F\rangle&=&1.802 \\ \end{array}$	$Al_1 - F_5 = 2 \times 1.808(6) F_5$	$F_9 - AI_1 - F_5 = 2 \times 89.8(4)$	$F_{9}-F_{5} = 2.512(6)$
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	$Al_1 - F_{11} = 2 \times 1.836(3) F_{11}$	$F_9 - Al_1 - F_{11} = 2 \times 90.2(4)$	$F_9 - F_{11} = 2.540(6)$
$F_{5}-AI_{1}-F_{11} = 2 \times 87.4(5) \qquad F_{5}-F_{11} = 2.518(7)$ $F_{5}-AI_{1}-F_{11} = 2 \times 92.6(5) \qquad F_{5}-F_{11} = 2.634(7)$ $AI_{1}-F_{5}-AI_{2} = 152.8(1)$ $AI_{1}-F_{11}-AI_{3} = 153.2(3)$ $AI_{2}^{3+} \text{ octahedron}$ $AI_{2}-F_{13}^{*} = 1.788(4)$ $AI_{2}-F_{6}^{*} = 1.789(4)$ $AI_{2}-F_{6}^{*} = 1.796(4)$ $AI_{2}-F_{3}^{*} = 1.801(4)$ $AI_{2}-F_{5} = 1.812(10)$ $\langle AI_{2}-F \rangle = 1.799$ $AI_{3}^{3+} \text{ octahedron}$ $AI_{3}-F_{2}^{*} = 1.744(10)$ $AI_{3}-F_{4}^{*} = 1.796(2)$ $AI_{3}-F_{12}^{*} = 1.801(3)$ $AI_{3}-F_{1}^{*} = 1.808(8)$ $AI_{3}-F_{1}^{*} = 1.822(6)$ $AI_{3}-F_{1} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$	$\langle AI_1 - F \rangle = 1.798 F$	$F_9 - AI_1 - F_{11} = 2 \times 89.8(4)$	$F_9 - F_{11} = 2.531(6)$
$F_{5}-AI_{1}-F_{11} = 2 \times 92.6(3) F_{5}-F_{11} = 2.634(7)$ $AI_{1}-F_{5} - AI_{2} = 152.8(1)$ $AI_{1}-F_{11}-AI_{3} = 153.2(3)$ $AI_{2}^{3+} \text{ octahedron}$ $AI_{2}-F_{13}^{*} = 1.788(4)$ $AI_{2}-F_{6}^{*} = 1.789(4)$ $AI_{2}-F_{6}^{*} = 1.796(4)$ $AI_{2}-F_{3}^{*} = 1.801(4)$ $AI_{2}-F_{3}^{*} = 1.807(8)$ $AI_{2}-F_{5} = 1.812(10)$ $\langle AI_{2}-F \rangle = 1.799$ $AI_{3}^{3+} \text{ octahedron}$ $AI_{3}-F_{2}^{*} = 1.744(10)$ $AI_{3}-F_{4}^{*} = 1.796(2)$ $AI_{3}-F_{12}^{*} = 1.801(3)$ $AI_{3}-F_{1}^{*} = 1.808(8)$ $AI_{3}-F_{1}^{*} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$	I	$F_{5}-AI_{1}-F_{11} = 2 \times 87.4(5)$	$F_5 - F_{11} = 2.518(7)$
$AI_{1}-F_{5} - AI_{2} = 152.8(1)$ $AI_{1}-F_{11}-AI_{3} = 153.2(3)$ $AI_{2}^{3+} \text{ octahedron}$ $AI_{2}-F_{13}^{*} = 1.788(4)$ $AI_{2}-F_{6}^{*} = 1.789(4)$ $AI_{2}-F_{6}^{*} = 1.796(4)$ $AI_{2}-F_{3}^{*} = 1.801(4)$ $AI_{2}-F_{3}^{*} = 1.807(8)$ $AI_{2}-F_{5} = 1.812(10)$ $\langle AI_{2}-F \rangle = 1.799$ $AI_{3}^{3+} \text{ octahedron}$ $AI_{3}-F_{2}^{*} = 1.744(10)$ $AI_{3}-F_{4}^{*} = 1.796(2)$ $AI_{3}-F_{12}^{*} = 1.801(3)$ $AI_{3}-F_{1}^{*} = 1.808(8)$ $AI_{3}-F_{1}^{*} = 1.822(6)$ $AI_{3}-F_{1} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$	H	$F_5 - AI_1 - F_{11} = 2 \times 92.6(5)$	$F_5 - F_{11} = 2.634(7)$
$AI_{1}-F_{11}-AI_{3} = 153.2(3)$ $AI_{2}^{3+} \text{ octahedron}$ $AI_{2}-F_{13}^{*} = 1.788(4)$ $AI_{2}-F_{6}^{*} = 1.789(4)$ $AI_{2}-F_{6}^{*} = 1.796(4)$ $AI_{2}-F_{3}^{*} = 1.801(4)$ $AI_{2}-F_{3}^{*} = 1.807(8)$ $AI_{2}-F_{5} = 1.812(10)$ $\langle AI_{2}-F \rangle = 1.799$ $AI_{3}^{3+} \text{ octahedron}$ $AI_{3}-F_{2}^{*} = 1.744(10)$ $AI_{3}-F_{4}^{*} = 1.796(2)$ $AI_{3}-F_{12}^{*} = 1.801(3)$ $AI_{3}-F_{1}^{*} = 1.808(8)$ $AI_{3}-F_{1}^{*} = 1.822(6)$ $AI_{3}-F_{1} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$	А	$l_1 - F_5 - Al_2 = 152.8(1)$	
$Al_{2}^{3+} \text{ octahedron}$ $Al_{2}-F_{13}^{*} = 1.788(4)$ $Al_{2}-F_{6}^{*} = 1.789(4)$ $Al_{2}-F_{10}^{*} = 1.796(4)$ $Al_{2}-F_{3}^{*} = 1.801(4)$ $Al_{2}-F_{3}^{*} = 1.807(8)$ $Al_{2}-F_{5} = 1.812(10)$ $\langle Al_{2}-F \rangle = 1.799$ $Al_{3}^{3+} \text{ octahedron}$ $Al_{3}-F_{2}^{*} = 1.744(10)$ $Al_{3}-F_{4}^{*} = 1.796(2)$ $Al_{3}-F_{12}^{*} = 1.801(3)$ $Al_{3}-F_{1}^{*} = 1.808(8)$ $Al_{3}-F_{1}^{*} = 1.822(6)$ $Al_{3}-F_{1} = 1.838(7)$ $\langle Al_{3}-F \rangle = 1.802$	А	$I_1 - F_{11} - AI_3 = 155.2(3)$	
$AI_{2}-F_{13}^{*} = 1.788(4)$ $AI_{2}-F_{6}^{*} = 1.789(4)$ $AI_{2}-F_{10}^{*} = 1.796(4)$ $AI_{2}-F_{3}^{*} = 1.801(4)$ $AI_{2}-F_{8}^{*} = 1.807(8)$ $AI_{2}-F_{5} = 1.812(10)$ $\langle AI_{2}-F \rangle = 1.799$ $AI_{3}^{3+} \text{ octahedron}$ $AI_{3}-F_{2}^{*} = 1.744(10)$ $AI_{3}-F_{4}^{*} = 1.796(2)$ $AI_{3}-F_{12}^{*} = 1.801(3)$ $AI_{3}-F_{1}^{*} = 1.808(8)$ $AI_{3}-F_{1}^{*} = 1.808(8)$ $AI_{3}-F_{1}^{*} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$		Al_2^{3+} octahedron	
$AI_{2}-F_{6}^{*} = 1.789(4)$ $AI_{2}-F_{10}^{*} = 1.796(4)$ $AI_{2}-F_{3}^{*} = 1.801(4)$ $AI_{2}-F_{8}^{*} = 1.807(8)$ $AI_{2}-F_{5} = 1.812(10)$ $\langle AI_{2}-F \rangle = 1.799$ $AI_{3}^{3+} \text{ octahedron}$ $AI_{3}-F_{2}^{*} = 1.744(10)$ $AI_{3}-F_{4}^{*} = 1.796(2)$ $AI_{3}-F_{12}^{*} = 1.801(3)$ $AI_{3}-F_{7}^{*} = 1.808(8)$ $AI_{3}-F_{1}^{*} = 1.822(6)$ $AI_{3}-F_{11} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$		$AI_2 - F_{13}^* = 1.788(4)$	
$AI_2-F_{10}^* = 1.796(4)$ $AI_2-F_3^* = 1.801(4)$ $AI_2-F_8^* = 1.807(8)$ $AI_2-F_5 = 1.812(10)$ $\langle AI_2-F \rangle = 1.799$ $AI_3^{3+} \text{ octahedron}$ $AI_3-F_2^* = 1.744(10)$ $AI_3-F_4^* = 1.796(2)$ $AI_3-F_{12}^* = 1.801(3)$ $AI_3-F_7^* = 1.808(8)$ $AI_3-F_1^* = 1.822(6)$ $AI_3-F_{11} = 1.838(7)$ $\langle AI_3-F \rangle = 1.802$		$Al_2 - F_6^* = 1.789(4)$	
$AI_2-F_3^* = 1.801(4)$ $AI_2-F_8^* = 1.807(8)$ $AI_2-F_5 = 1.812(10)$ $\langle AI_2-F \rangle = 1.799$ $AI_3^{3+} \text{ octahedron}$ $AI_3-F_2^* = 1.744(10)$ $AI_3-F_4^* = 1.796(2)$ $AI_3-F_{12}^* = 1.801(3)$ $AI_3-F_7^* = 1.808(8)$ $AI_3-F_1^* = 1.822(6)$ $AI_3-F_{11} = 1.838(7)$ $\langle AI_3-F \rangle = 1.802$		$Al_2 - F_{10}^* = 1.796(4)$	
$AI_{2}-F_{8}^{*} = 1.80/(8)$ $AI_{2}-F_{5} = 1.812(10)$ $\langle AI_{2}-F \rangle = 1.799$ $AI_{3}^{3+} \text{ octahedron}$ $AI_{3}-F_{2}^{*} = 1.744(10)$ $AI_{3}-F_{4}^{*} = 1.796(2)$ $AI_{3}-F_{12}^{*} = 1.801(3)$ $AI_{3}-F_{7}^{*} = 1.808(8)$ $AI_{3}-F_{1}^{*} = 1.822(6)$ $AI_{3}-F_{11} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$		$AI_2 - F_3^* = 1.801(4)$	
$A_{12}-F_{5} = 1.812(10)$ $\langle Al_{2}-F \rangle = 1.799$ $Al_{3}^{3+} \text{ octahedron}$ $Al_{3}-F_{2}^{*} = 1.744(10)$ $Al_{3}-F_{4}^{*} = 1.796(2)$ $Al_{3}-F_{12}^{*} = 1.801(3)$ $Al_{3}-F_{7}^{*} = 1.808(8)$ $Al_{3}-F_{7}^{*} = 1.822(6)$ $Al_{3}-F_{11} = 1.838(7)$ $\langle Al_{3}-F \rangle = 1.802$		$Al_2 - F_8^* = 1.80/(8)$	
$AI_{3}^{3+} \text{ octahedron}$ $AI_{3}^{-}F_{2}^{*} = 1.744(10)$ $AI_{3}-F_{4}^{*} = 1.796(2)$ $AI_{3}-F_{12}^{*} = 1.801(3)$ $AI_{3}-F_{7}^{*} = 1.808(8)$ $AI_{3}-F_{7}^{*} = 1.822(6)$ $AI_{3}-F_{11} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$	/	$AI_2 - F_5 = 1.812(10)$	
$AI_{3}^{*+} \text{ octahedron}$ $AI_{3}-F_{2}^{*} = 1.744(10)$ $AI_{3}-F_{4}^{*} = 1.796(2)$ $AI_{3}-F_{12}^{*} = 1.801(3)$ $AI_{3}-F_{7}^{*} = 1.808(8)$ $AI_{3}-F_{1}^{*} = 1.822(6)$ $AI_{3}-F_{11} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$	١	Al2-17 ~ 1.733	
$A_{13}-F_{2} = 1.744(10)$ $A_{13}-F_{4}^{*} = 1.796(2)$ $A_{13}-F_{12}^{*} = 1.801(3)$ $A_{13}-F_{7}^{*} = 1.808(8)$ $A_{13}-F_{1}^{*} = 1.822(6)$ $A_{13}-F_{11} = 1.838(7)$ $\langle A_{13}-F \rangle = 1.802$		AI_3^{2+} octahedron	
$A_{13}-F_4 = 1.750(2)$ $A_{13}-F_{12}^* = 1.801(3)$ $A_{13}-F_7^* = 1.808(8)$ $A_{13}-F_1^* = 1.822(6)$ $A_{13}-F_{11} = 1.838(7)$ $\langle A_{13}-F \rangle = 1.802$		$A_{13}-F_2^+ = 1.794(10)$	
$AI_{3}-F_{12} = 1.808(8)$ $AI_{3}-F_{7}^{*} = 1.822(6)$ $AI_{3}-F_{11} = 1.838(7)$ $\langle AI_{3}-F\rangle = 1.802$		$A_{13} - F_4^2 = 1.790(2)$ $A_{1-} - F_{-} = 1.801(3)$	
$AI_{3}-F_{1}^{*} = 1.822(6)$ $AI_{3}-F_{11} = 1.838(7)$ $\langle AI_{3}-F \rangle = 1.802$		$A_{1} - F_{12} = 1.001(3)$ $A_{1} - F_{2}^{*} = 1.808(8)$	
$AI_{3}-F_{11} = 1.838(7)$ (AI_{3}-F) = 1.802		$Al_{2}-F_{1}^{*} = 1.822(6)$	
$\langle Al_3 - F \rangle = 1.802$		$A_{13} - F_{11} = 1.838(7)$	
	($\langle Al_3 - F \rangle = 1.802$	

TABLE III—Continued

Na ⁺ polyhedron [8]			
$Na_{1}-F_{10} = 2 \times 2393(3) F_{10}-Na_{1}-F_{10} = 2 \times 853(4) F_{10}-F_{11} = 3255(7)$			
$Na_{11}F_{10} = 2 \times 2410(3) F_{10} Na_{11}F_{12} = 2 \times 60.3(4) F_{10}F_{12} = 3.255(7)$			
$Na_1 = 1_1 = 2 \times 2.410(3) = 1_{10} = Na_1 = 1_6 = 2 \times 00.3(3) = 1_{10} = 1_6 = 2.523(6)$ $Na_2 = E_1 = 2 \times 2.615(8) = 1_{10} = Na_2 = E_1 = 2 \times 75.3(4) = E_2 = 2.121(6)$			
$N_{0} = F_{0} = 2 \times 2.005(0) F_{10} = N_{0} = F_{0} = 2 \times 75.0(4) F_{10} = F_{0} = 3.121(0)$			
$Na_1 - \Gamma_7 = 2 \times 2.704(4) \Gamma_{12} - Na_1 - \Gamma_6 = 2 \times 75.0(4) \Gamma_{12} - \Gamma_6 = 3.085(6)$			
$(Na_1-F) = 2.530$ $F_{12}-Na_1-F_7 = 2 \times 57.8(5)$ $F_{12}-F_7 = 2.484(9)$			
$F_6 - Na_1 - F_7 = 2 \times 68.8(4) F_6 - F_7 = 3.007(7)$			
Na_2^+ polyhedron [8]			
$Na_{2}-F_{12} = 2 \times 2.270(4)$			
$Na_{2} = 12 \times 2.285(10)$			
$Na_2 = 16 = 2 \times 2.205(10)$ No. E = 2 × 2.42(8)			
$1(a_2-1)_5 = 2 \times 2.003(8)$			
$Na_2 - F_9 = 2 \times 2.848(5)$			
$\langle Na_2 - F \rangle = 2.517$			
Na_3^+ polyhedron [8]			
$Na_3 - F_{10} = 2 \times 2.272(4)$			
$Na_3 - F_7 = 2 \times 2.276(10)$			
$Na_3 - F_{11} = 2 \times 2.702(9)$			
$Na_3 - F_9 = 2 \times 2.797(5)$			
$\langle Na_3 - F \rangle = 2.512$			

" Estimated standard deviations are given in parentheses.

* Terminal fluorine.

other sodium atoms (Na₍₂₎ and Na₍₃₎) are inserted between two parallel chains either at level $z \simeq 0$ (Fig. 3) or at level $z \simeq \frac{1}{2}$ whereas



FIG. 2. (100) projection of the Na₃Sr₄Al₃F₂₆ structure drawn by means of the STRUPLO program (8). Shaded Al₃F₂₆ pentamers are those centered at x = 0; unshaded ones are centered at $x = \frac{1}{2}$. Na and Sr are represented by small and large circles, respectively (Na₍₁₎ black small circles).

the strontium atoms $(Sr_{(1)} \text{ and } Sr_{(2)})$ are located between the 90° rotated chains (see Fig. 2).

One possible explanation of the easy twinning observed for this compound is il-



FIG. 3. (001) projection of the Na₃Sr₄Al₅F₂₆ structure with -0.25 < z < 0.25. Two Na₍₂₎ and Na₍₃₎ polyhedra are drawn. Na and Sr symbols are defined in Fig. 2.



FIG. 4. (001) projection of the Na₃Sr₄Al₅F₂₆ structure with 0.25 < z < 0.75. Symbols as in Fig. 2.

lustrated in Fig. 5. Two crystals can share a common plane perpendicular to the *c*-axis in which the Al₅F₂₆ blocks at z = 0 from a domain A become the Al₅F₂₆ blocks at $z = \frac{1}{2}$ from a domain B. Such a twinning only involves small shifts of atoms (0.14 Å between Al₍₂₎ and Al₍₃₎, 0.12 Å between Na₍₂₎ and Na₍₃₎).

The mean Al-F observed distances (1.80



FIG. 5. View of a possible twinning between two crystals A and B. Symbols as in Fig. 2. Shaded Al₅F₂₆ blocks are centered at x = 0 (A) and y = 0 (B); unshaded ones are centered at $x = \frac{1}{2}$ (A) and $y = \frac{1}{2}$ (B).

Å) for the three octahedra are in good agreement and close to the sum of Shannon's radii (9) (1.82 Å); the smaller Al-F bonds always correspond to terminal fluorines (see Table III).

To our knowledge, the [Al₅F₂₆]¹¹⁻ pentamer has not been encountered in fluoaluminates. However the corner connection mode between the central octahedron and the four others, rotated by 90° (see Fig. 1), is observed in the $[Al_3F_{14}]^{5-}$ layers of the Chiolite structure $Na_5Al_3F_{14}$ (10, 11). Indeed, in Na₃Sr₄Al₅F₂₆ there exists isolated octahedra pentamers $[Al_5F_{26}] = AlF_4$ $[Al_4F_{22}]$ where AlF₄ is the central octahedron and in Na₅Al₃F₁₄ these octahedra pentamers undergo a condensation by sharing the external octahedra, resulting in a layer $AlF_4[Al_2F_{10}] = Al_3F_{14}$. A study of the homologous compounds with $M^{\text{III}} = 3d$ transition metal is in progress.

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