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OPTICAL PROPERTIES AND X-RAY DIFFRACTION
DATA FOR SOME INORGANIC FLUORIDE
AND CHLORIDE COMPOUNDS

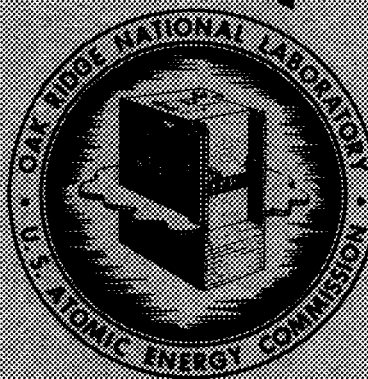
H. Insley
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CHEMISTRY DIVISION

and

METALLURGY DIVISION

OPTICAL PROPERTIES AND X-RAY DIFFRACTION DATA
FOR SOME INORGANIC FLUORIDE AND CHLORIDE COMPOUNDS

H. Insley, Consultant
T. N. McVay, Consultant
R. E. Thoma, Chemistry Division
G. D. White, Metallurgy Division

Date Issued

OCT 23 1958

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OPTICAL PROPERTIES AND X-RAY DIFFRACTION DATA
FOR SOME INORGANIC FLUORIDE AND CHLORIDE COMPOUNDS

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G. D. White, Metallurgy Division

ABSTRACT

Optical properties and X-ray diffraction data are listed for various inorganic fluoride and chloride compounds. This publication extends and replaces ORNL-1712, Properties of Some Inorganic Fluoride and Chloride Compounds, by T. N. McVay and G. D. White.

INTRODUCTION

Optical and X-ray diffraction data have been collected for many compounds whose existence was not known prior to their discovery incidental to the phase equilibrium studies made in the High Temperature Section of the Chemistry Division. A few compounds are listed and mentioned in the footnotes whose initial discovery was not made at ORNL; however, the original optical measurements on these compounds were made by H. Insley, T. N. McVay, and G. D. White of the Ceramics Laboratory, Metallurgy Division.

The standard X-ray diffraction patterns included herein were derived, in general, from the same samples on which the optical data were taken. Standard patterns were made from powder samples with a Norelco-Phillips high angle diffractometer, using Cu K α filtered radiation from a General Electric CA-7 X-ray tube. The diffractometer was equipped with a Geiger Muller tube counting arrangement. The X-ray data have not been corrected for absorption. Values for interplanar distances (d, measured in Angstrom units) and relative intensities of diffracting maxima conform to the conventions used in the ASTM X-ray diffraction data cards.

The refractive indices of the compounds included are believed to be precise to ± 0.003 ; the optic angles of biaxial crystals were estimated.

This publication is divided into Part I (optical properties) and Part II (X-ray diffraction data). The three strongest X-ray lines accompany the optical data of each compound for which ASTM X-ray diffraction data are not available, if those X-ray data were derived at ORNL. X-ray diffraction data in Part II are separated according to the purity of the samples used for standards. Patterns for the compounds in the first section were derived from single-phase samples of known chemical analysis which had met optical standards. In the second section are listed data on compounds whose purity has not been absolutely established.

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PART I

OPTICAL PROPERTIES

Ammonium beryllium fluoride, $2 \text{ NH}_4 \cdot \text{BeF}_2$

Uniaxial +
 $n = 1.319$
Low birefringence
Colorless
Questionable. National Research Council Bulletin 118 describes it as rhombic.

Beryllium fluoride, BeF_2

Uniaxial +
 $n = 1.325$
Low birefringence estimated .006
Quartz form
Colorless
Sample prepared at Mound Laboratory.

Beryllium lead fluoride, $\text{BeF}_2 \cdot \text{PbF}_2$

Biaxial - $2V = 70^\circ$
 $\alpha = 1.602$ $\gamma = 1.627$
Colorless

Cesium beryllium fluoride, $2 \text{ CsF} \cdot \text{BeF}_2$

$n = 1.452$
Very low birefringence
Colorless.

Cesium beryllium fluoride, $\text{CsF} \cdot \text{BeF}_2$

$n = 1.382$
Low birefringence
Length slow. Parallel extinction.
Colorless.

Cesium lanthanum fluoride, $3 \text{ CsF} \cdot \text{LaF}_3$

Cubic
 $n = 1.462$
Colorless
X-ray lines: 3.49, 2.478, 2.021.

Cesium uranium fluoride, $\text{CsF} \cdot \text{UF}_4$

Biaxial + $2V = 45^\circ$
 $\alpha = 1.553$ $\gamma = 1.560$
Polysynthetic twinning $X_{Ac} = 10^\circ$ $Z = \text{sky blue}$
 $X = \text{greenish blue}$
X-ray lines: 7.31, 4.00, 3.62

Cesium uranium fluoride, $2 \text{ CsF} \cdot \text{UF}_4$

Biaxial +	$2V = 45^\circ$
$\alpha = 1.516$	$\gamma = 1.524$
X = light greenish blue	Z = light blue
X-ray lines: 6.19, 3.55, 3.44.	

Cesium zinc fluoride, $2 \text{ CsF} \cdot \text{ZnF}_2$

Biaxial +	$2V = \text{small}$
$\alpha = 1.446$	$\gamma = 1.458$
Colorless	

Cesium zirconium fluoride, $\text{CsF} \cdot \text{ZrF}_4$

Biaxial -	$2V = 20^\circ - 45^\circ$ (varies)
$\alpha = 1.464$	$\gamma = 1.476$
Colorless	
X-ray lines: 3.73, 3.62, 3.26	

Cesium zirconium fluoride, $2 \text{ CsF} \cdot \text{ZrF}_4$

Uniaxial -	$\epsilon = 1.460$
$\omega = 1.482$	
Colorless	
X-ray lines: 3.73, 3.20, 2.430.	

Chromium fluoride, CrF_2

Biaxial +	$2V = 10^\circ$
Monoclinic	$X_{Ac} = 38^\circ$
$\alpha = 1.511$	$\gamma = 1.525$
Gray green	
X-ray lines: 3.53, 2.97, 2.805	

Iron fluoride, FeF_2

Uniaxial +	
$\omega = 1.524$	$\epsilon = 1.540$
Brown	

Iron zirconium fluoride, $\text{FeF}_2 \cdot \text{ZrF}_4$

Cubic	
$n = 1.432$	
X-ray lines: 4.04, 2.016, 1.805	

Lanthanum fluoride, LaF_3

Uniaxial -
Hexagonal
 $\omega = 1.605$
Length fast
Prismatic
Colorless.

$$\epsilon = 1.594$$

Lanthanum zirconium uranium fluoride, $\text{LaF}_3 \cdot 6\text{ZrF}_4 \cdot \text{UF}_4$

Biaxial +
 $\alpha = 1.528$
Light green.

$$2V = 70^\circ$$
$$\gamma = 1.545$$

Lead uranium fluoride, $\text{PbF}_2 \cdot \text{UF}_4$

Uniaxial -
 $\omega = 1.750$
Green.

$$\epsilon = 1.730$$

Lead uranium fluoride, 6 $\text{PbF}_2 \cdot \text{UF}_4$

Cubic
 $n = 1.77$
Light blue.

Lithium beryllium fluoride, 2 $\text{LiF} \cdot \text{BeF}_2$

Uniaxial +
 $\omega = 1.312$
Colorless.

$$\epsilon = 1.319$$

Lithium cesium fluoride, $\text{LiF} \cdot \text{CsF}$

Biaxial +
 $n = 1.458$
Estimated birefringence 0.006
Colorless

$$2V = \text{small}$$

Lithium chromium fluoride, 3 $\text{LiF} \cdot \text{CrF}_3$

Biaxial -
 $\alpha = 1.444$
Green

$$2V = 40^\circ$$
$$\gamma = 1.464$$

X-ray lines: 4.29, 4.16, 2.176.

Lithium rubidium fluoride, $\text{LiF} \cdot \text{RbF}$

Biaxial +
Orthorhombic
 $n = 1.396$
Low birefringence
Colorless.

Lithium sodium beryllium fluoride, $\text{LiF} \cdot 2\text{NaF} \cdot 2\text{BeF}_2$

Uniaxial -
 $n = 1.311$
Low birefringence
Colorless.

Lithium uranium fluoride, $4\text{LiF} \cdot \text{UF}_4$

Biaxial +	$2V = 45^\circ$
$\alpha = 1.460$	$\gamma = 1.472$
X = light green	Z = dark green
X-ray lines: 5.13, 4.93, 4.44.	

Lithium uranium fluoride, $7\text{LiF} \cdot 6\text{UF}_4$

Uniaxial -	
$\omega = 1.554$	$\epsilon = 1.551$
Deep green	
X-ray lines: 5.24, 3.33, 2.99.	

Lithium uranium fluoride, $\text{LiF} \cdot 4\text{UF}_4$

Biaxial -	$2V = 10^\circ$
$\alpha = 1.584$	$\gamma = 1.600$
Yellowish green	
X-ray lines: 4.25, 3.78, 3.52.	

Lithium zirconium fluoride, $\text{LiF} \cdot \text{ZrF}_4$

Biaxial +	$2V = 30^\circ$
$\alpha = 1.468$	$\gamma = 1.476$
Colorless	
Quench determinations show this phase to have compositions $3\text{LiF} \cdot 4\text{ZrF}_4$ with biaxial +.	
X-ray lines: 3.90, 3.33, 3.16.	

Lithium zirconium fluoride, $3\text{LiF} \cdot 4\text{ZrF}_4$

Biaxial +	$2V = 30^\circ$
$\alpha = 1.463$	$\gamma = 1.473$
Colorless	
X-ray lines: 3.90, 3.33, 3.16.	

Lithium zirconium fluoride, $2 \text{ LiF} \cdot \text{ZrF}_4$

Uniaxial +
 $\omega = 1.468$ $\epsilon = 1.478$
Colorless
X-ray lines: 4.29, 3.15, 2.19

Lithium zirconium fluoride, $3 \text{ LiF} \cdot \text{ZrF}_4$

Biaxial - $2V = 30^\circ$
 $\alpha = 1.445$ $\gamma = 1.465$
Colorless
X-ray lines: 5.49, 4.88, 2.07

Manganese fluoride, MnF_2

Uniaxial +
 $\omega = 1.476$ $\epsilon = 1.504$
X = colorless $Z = \text{gray}$

Nickel fluoride, NiF_2

Uniaxial +
 $\omega = 1.526$ $\epsilon = 1.560$
Light greenish yellow.

Nickel zirconium fluoride, $\text{NiF}_2 \cdot \text{ZrF}_4$

$n = 1.442$
Very low birefringence
X-ray lines: 3.91, 1.964, 1.767.

Potassium aluminum fluoride, $3 \text{ KF} \cdot \text{AlF}_3$

Cubic
 $n = 1.376$
Colorless.

Potassium beryllium fluoride, $3 \text{ KF} \cdot \text{BeF}_2$

Uniaxial +
 $\omega = 1.357$ $\epsilon = 1.366$
Colorless
X-ray lines: 2.98, 2.39, 2.27.

Potassium beryllium fluoride, $2 \text{ KF} \cdot \text{BeF}_2$

Biaxial + $2V = 30^\circ$
 $\alpha = 1.357$ $\gamma = 1.366$
Probably monoclinic
 $X_{Ac} = 40^\circ$
Colorless.

Potassium beryllium fluoride, $\text{KF} \cdot \text{BeF}_2$

Biaxial - $2V = 45^\circ$
 $\alpha = 1.319$ $\gamma = 1.323$
Colorless
X-ray lines: 5.99, 3.33, 3.01.

Potassium beryllium fluoride, $\text{KF} \cdot 2\text{BeF}_2$

Uniaxial -
 $\omega = 1.319$ $\epsilon = 1.312$
Colorless
X-ray lines: 3.31, 3.00, 2.29.

Potassium chromium fluoride, $3 \text{KF} \cdot \text{CrF}_3$

Cubic
 $n = 1.422$
Green
X-ray lines: 4.95, 3.03, 2.35.

Potassium fluoride acid, $\text{KF} \cdot \text{HF}$

Uniaxial -. Some crystals have a small optic angle.
 $\omega = 1.354$ $\epsilon = 1.331$

Potassium iron chloride, $\text{KCl} \cdot \text{FeCl}_2$

Biaxial + $2V = 20^\circ$
 $\alpha = 1.700 \pm 0.005$ $\gamma = 1.740 \pm 0.005$
Colorless.

Potassium iron chloride, $2 \text{KCl} \cdot \text{FeCl}_2$

Uniaxial +
 $\omega = 1.600$ $\epsilon = 1.636$
Colorless.

Potassium lanthanum fluoride, $\text{KF} \cdot \text{LaF}_3$

Uniaxial +
 $\omega = 1.493$ $\epsilon = 1.510$
Colorless
X-ray lines: 7.77, 2.747, 1.857.

Potassium nickel fluoride, $2 \text{KF} \cdot \text{NiF}_2$

Uniaxial -
Tetragonal
 $\omega = 1.434$ $\epsilon = 1.426$
Yellow
X-ray lines: 6.51, 2.94, 2.173.

Potassium sodium beryllium fluoride, $\text{KF} \cdot \text{NaF} \cdot \text{BeF}_2$

Biaxial + 2V = small
n = 1.343
Low birefringence
Colorless
X-ray lines: 2.786, 2.367, 1.995.

Potassium sodium iron fluoride, $2 \text{KF} \cdot \text{NaF} \cdot \text{FeF}_3$

Cubic
n = 1.414
Colorless

Potassium sodium zirconium fluoride, $3 \text{KF} \cdot 3\text{NaF} \cdot 2\text{ZrF}_4$

Biaxial + 2V = 30°
 $\alpha = 1.410$ $\gamma = 1.421$
Colorless
X-ray lines: 4.90, 4.09, 2.97.

Potassium sodium zirconium fluoride, $\text{KF} \cdot \text{NaF} \cdot \text{ZrF}_4$

Biaxial - 2V = 60°
 $\alpha = 1.378$ $\gamma = 1.385$
Colorless
Often fibrous or prismatic
X-ray lines: 4.85, 4.09, 3.34

Potassium sodium zirconium fluoride, $3\text{KF} \cdot 2\text{NaF} \cdot 5\text{ZrF}_4$

Biaxial - 2V = about 80°
 $\alpha = 1.478$ $\gamma = 1.488$
Colorless
Probably monoclinic
Marked cleavage; Z Δ elong. about 7°
X-ray lines: 8.51, 7.70, 3.86.

Potassium tellurium fluoride, $\text{KTeF}_5 \cdot \text{H}_2\text{O}$

Biaxial + 2V = 30°
 $\alpha = 1.436$ $\gamma = 1.460$
Colorless
X-ray lines: 5.64, 4.27, 3.575.

Potassium thorium fluoride, $3 \text{KF} \cdot \text{ThF}_4$

Cubic
n = 1.424
Colorless

Potassium uranium chloride, $\text{KCl} \cdot \text{UCl}_4$

Biaxial +	$2V = \text{small}$	
$\alpha = 1.692$	$\beta = 1.705$	$\gamma = 1.759$
X = gray	Z = blue green	

Potassium uranium fluoride, $7 \text{KF} \cdot 6 \text{UF}_4$

Uniaxial -
 $\omega = 1.510$ $\epsilon = 1.504$
Green
X-ray lines: 4.82, 3.44, 1.793

Potassium uranium fluoride, $\text{KF} \cdot \text{UF}_3$

Isomorphous with $\text{NaF} \cdot \text{UF}_3$
Similar optical properties.

Potassium uranium fluoride, $\text{KF} \cdot 2\text{UF}_4$

Biaxial -	$2V = 15^\circ$
$\alpha = 1.520$	$\gamma = 1.584$
Green.	

Potassium uranium fluoride, $2 \text{KF} \cdot \text{UF}_4$

Uniaxial +	
$\omega = 1.484$	$\epsilon = 1.512$
Light olive drab.	

Potassium zinc fluoride, $\text{KF} \cdot \text{ZnF}_2$

Cubic
 $n = 1.462$
Colorless.

Potassium zinc fluoride, $2 \text{KF} \cdot \text{ZnF}_2$

Uniaxial -	
$\omega = 1.416$	$\epsilon = 1.410$

Potassium zirconium fluoride, $2 \text{KF} \cdot \text{ZrF}_4$

"Low temperature" form
Biaxial + $2V = 10^\circ$
 $\alpha = 1.412$ $\gamma = 1.424$
Polysynthetic twinning frequent
Colorless.

Potassium zirconium fluoride, $\alpha\text{KF}\cdot\text{ZrF}_4$

Biaxial - $2V = 80^\circ$
 $\alpha = 1.412$ $\gamma = 1.428$
Colorless
X-ray lines: 5.83, 4.40, 3.86.

Potassium zirconium fluoride, $\beta\text{KF}\cdot\text{ZrF}_4$

Biaxial + $2V = 75^\circ$
 $\alpha = 1.488$ $\gamma = 1.504$
Colorless
X-ray lines: 6.32, 3.29, 3.15.

Rubidium beryllium fluoride, $\text{RbF}\cdot 2\text{BeF}_2$

Biaxial - $2V = 70^\circ$
 $n = 1.333$
Birefringence about 0.008
Colorless

Rubidium cerium fluoride, $\text{RbF}\cdot\text{CeF}_3$

Biaxial + $2V = 75^\circ$
 $\alpha = 1.500$ $\gamma = 1.520$

Rubidium lanthanum fluoride, $\text{RbF}\cdot\text{LaF}_3$

Biaxial + $2V = 70^\circ$
 $\alpha = 1.498$ $\gamma = 1.519$
Colorless
X-ray lines: 3.43, 2.25, 1.90.

Rubidium lanthanum fluoride, $3 \text{RbF}\cdot\text{LaF}_3$

Cubic
 $n = 1.424$
Colorless
X-ray lines: 3.30, 2.821, 3.11.

Rubidium sodium beryllium fluoride, $\text{RbF}\cdot 2\text{NaF}\cdot\text{BeF}_2$

Cubic
 $n = 1.374$
Colorless
X-ray lines: 2.99, 2.875, 2.494.

Rubidium sodium uranium fluoride, $\text{RbF}\cdot\text{NaF}\cdot\text{UF}_4$

Uniaxial +
 $\omega = 1.484$ $\epsilon = 1.486$
Anomalous purple interference color characteristic.
Pale green
X-ray lines: 8.12, 3.26, 2.034.

Rubidium uranium fluoride, 3 RbF·UF₄

Cubic
n = 1.438
Green
X-ray lines: 5.56, 3.40, 1.959.

Rubidium uranium fluoride, RbF·UF₄

Biaxial - 2V = 75°
 $\alpha = 1.514$ $\gamma = 1.528$
Polysynthetic twinning
Y_{Ac} = 20°
Lath-shaped crystals
X = green Z = blue
Marked dispersion of optic axes
X-ray lines: 6.86, 3.46, 3.43.

Rubidium uranium fluoride, 2 RbF·UF₄

Biaxial + 2V = 70°
 $\alpha = 1.473$ $\gamma = 1.487$
X = light green Z = light violet
Polysynthetic twinning common
X-ray lines: 6.03; 3.49, 2.008.

Rubidium uranium fluoride, 7 RbF·6 UF₄

Uniaxial -
 $\omega = 1.518$ $\epsilon = 1.512$
X-ray lines: 3.51, 2.140, 1.835.

Rubidium uranium fluoride, 2 RbF·3 UF₄

Biaxial - 2V = 60°
 $\alpha = 1.542$ $\gamma = 1.550$
Inclined extinction
Pleochroic, bluish green and pale violet-green
X-ray lines: 5.80, 3.50, 2.038.

Rubidium uranium fluoride, RbF·3UF₄

Biaxial + 2V = 70°
 $\alpha = 1.588$ $\gamma = 1.598$
Yellow green with slight dichroism
Strong dispersion of optic axes
Anomalous dispersion of birefringence in purplish red
X-ray lines: 3.52, 3.36, 2.002.

Rubidium uranium fluoride, $\text{RbF} \cdot 6\text{UF}_4$

Uniaxial -
Probably tetragonal
 $\omega = 1.596$ $\epsilon = 1.586$
Deep green
X-ray lines: 4.13, 3.47, 2.049

III

Rubidium uranium fluoride, $3\text{RbF} \cdot \text{UF}_3$

Cubic
 $n = 1.440$ approximate
Pinkish brown.

Rubidium zirconium fluoride, $3\text{RbF} \cdot \text{ZrF}_4$

Cubic
 $n = 1.420$
Colorless
X-ray lines: 3.290, 2.236, 1.990

Rubidium zirconium fluoride, $2 \text{RbF} \cdot \text{ZrF}_4$

Uniaxial - (low temperature form)
 $\omega = 1.440$ $\epsilon = 1.426$
Colorless
X-ray lines: 3.590, 3.080, 2.338.

Rubidium zirconium fluoride, $5 \text{RbF} \cdot 4\text{ZrF}_4$

Biaxial - $2V$ about 85°
 $\alpha = 1.442$ $\gamma = 1.452$
Colorless
X-ray lines: 3.44, 3.36, 3.29.

Rubidium zirconium fluoride, $\text{RbF} \cdot \text{ZrF}_4$

Biaxial - $2V =$ about 75°
 $\alpha = 1.490$ $\gamma = 1.502$
Elong. fast extinction about 2°
X-ray lines: 3.42, 3.36, 3.325.

Sodium beryllium fluoride, $\text{NaF} \cdot \text{BeF}_2$

Biaxial $2V =$ large
 $n = 1.312$
Low birefringence
Length slow
colorless

Sodium beryllium fluoride, $2 \text{ NaF} \cdot \text{BeF}_2$

Low temperature
Biaxial
 $n = 1.303$
Low birefringence
Yllc
Colorless
Sometimes twinned.

Sodium beryllium fluoride, $2 \text{ NaF} \cdot \text{BeF}_2$

High temperature form.
Cubic
 $n = 1.333$
Colorless.

Sodium cerium fluoride, $\text{NaF} \cdot \text{CeF}_3$

Uniaxial +
 $\omega = 1.493$ $\epsilon = 1.514$
X-ray lines: 3.09, 2.57, 1.777.

Sodium chromium fluoride, $3 \text{ NaF} \cdot \text{CrF}_3$

Cubic
 $n = 1.411$
Green

Sodium fluoride acid, $\text{NaF} \cdot \text{HF}$

Uniaxial +
 $\omega = 1.261$ $\epsilon = 1.328$
Colorless

Sodium lanthanum fluoride, $\text{NaF} \cdot \text{LaF}_3$

Uniaxial +
 $\omega = 1.486$ $\epsilon = 1.500$
X-ray lines: 3.11, 3.09, 2.194.

Sodium thorium fluoride, $2 \text{ NaF} \cdot \text{ThF}_4$

Uniaxial +
 $\omega = 1.464$ $\epsilon = 1.496$
Colorless
X-ray lines: 5.17, 2.99, 1.742

Sodium uranium chloride, $2 \text{ NaCl} \cdot \text{UCl}_4$

Uniaxial -
 $\omega = 1.664$ $\epsilon = 1.652$
Pale green

Sodium uranium fluoride, $\text{NaF} \cdot \text{UF}_3$

Uniaxial +
 $\omega = 1.552$ $\epsilon = 1.564$
Dark blue
X-ray lines: 3.09, 2.179, 1.779.

Sodium uranium fluoride, $2 \text{ NaF} \cdot \text{UF}_4$

Uniaxial -
 $\omega = 1.495$ $\epsilon = 1.490$
Green
X-ray lines: 7.25, 4.28, 2.99.

Sodium uranium fluoride, $\beta 2$, $2 \text{ NaF} \cdot \text{UF}_4$

Uniaxial +
 $\omega = 1.484$ $\epsilon = 1.522$
X = greenish-tan $Z = \text{gray-tan}$

Sodium uranium fluoride, $3 \text{ NaF} \cdot \text{UF}_4$

Uniaxial -
 $\omega = 1.417$ $\epsilon = 1.411$
Greenish blue
X-ray lines: 5.15, 2.97, 2.102.

Sodium uranium fluoride, $5 \text{ NaF} \cdot 3 \text{ UF}_4$

Cubic
 $n = 1.475$
Green
X-ray lines: 3.19, 1.964, 1.684.

Sodium uranium fluoride, $\text{NaF} \cdot 2 \text{ UF}_4$

Biaxial - $2V = 60^\circ$
Orthorhombic
 $\alpha = 1.516$ $\gamma = 1.584$
Yellowish green
X-ray lines: 5.61, 3.26, 3.08.

Sodium uranium fluoride, $7 \text{ NaF} \cdot 6 \text{ UF}_4$

Uniaxial -

$\omega = 1.520$

$\epsilon = 1.512$

Green

X-ray lines: 4.32, 3.33, 3.25.

Sodium zinc fluoride, $2 \text{ NaF} \cdot \text{ZnF}_2$

Uniaxial -

Tetragonal

$\omega = 1.418$

$\epsilon = 1.410$

Colorless

Sodium zirconium fluoride, $3 \text{ NaF} \cdot 4 \text{ ZrF}_4$

Biaxial +

$2V = 30^\circ$

$\alpha = 1.420$

$\gamma = 1.432$

Colorless

X-ray lines: 4.15, 3.36, 2.074.

Sodium zirconium fluoride, $\text{NaF} \cdot \text{ZrF}_4$

Metastable phase

Uniaxial +

$\omega = 1.417$

$\epsilon = 1.446$

Colorless

X-ray lines: 3.37, 3.86, 2.09.

Sodium zirconium fluoride, $7 \text{ NaF} \cdot 6 \text{ ZrF}_4$

Uniaxial -

$\omega = 1.508$

$\epsilon = 1.500$

Indices depend on composition

Colorless

Some solid solution in this area

X-ray lines: 3.13, 1.92, 1.91.

Sodium zirconium fluoride, $2 \text{ NaF} \cdot \text{ZrF}_4$

" β_1 " form

Uniaxial +

$\omega = 1.406$

$\epsilon = 1.408$

Colorless

Partially miscible with $3 \text{ NaF} \cdot \text{ZrF}_4$

X-ray lines: 5.15, 3.09, 1.890.

Sodium zirconium fluoride, $2 \text{ NaF} \cdot \text{ZrF}_4$

Biaxial - $2V = 75^\circ$
 $\alpha = 1.412$ $\gamma = 1.419$
Colorless
" β_2 " form
X-ray lines: 5.47, 3.11, 1.912.

Sodium zirconium fluoride, $2 \text{ NaF} \cdot \text{ZrF}_4$

" β_3 " form, stable $500-530^\circ$ approx.
Uniaxial +
 $\omega = 1.376$ $\epsilon = 1.386$
Colorless
X-ray lines: 4.55, 2.893, 1.894.

Sodium zirconium fluoride, $2 \text{ NaF} \cdot \text{ZrF}_4$

" β_4 " form
Biaxial + $2V = 75^\circ$
 $\alpha = 1.408$ $\gamma = 1.412$
Colorless
X-ray lines: 5.12, 3.83, 3.25.

Sodium zirconium fluoride, $2 \text{ NaF} \cdot \text{ZrF}_4$

" γ " form
Biaxial - $2V > 70^\circ$
 $\alpha = 1.420$ $\gamma = 1.429^\circ$
Colorless
Polysynthetic twinning common
X-ray lines: 4.98, 4.19, 3.07.

Sodium zirconium fluoride, $3 \text{ NaF} \cdot \text{ZrF}_4$

Uniaxial -
 $\omega = 1.386$ $\epsilon = 1.381$
Colorless
X-ray lines: 4.75, 3.06, 1.87.

Thorium fluoride, ThF_4

Biaxial - $2V = 60^\circ$
 $\alpha = 1.500$ $\gamma = 1.534$
Colorless

Uranium chloride, UCl_3

Uniaxial probably -
High n 2.04
Dark brownish red

Low n 1.94

Uranium chloride, UCl_4

Uniaxial -
 $\omega = 2.03$
 $X =$ light brownish green

$\epsilon = 1.95$
 $Z =$ greenish brown

Yttrium fluoride, YF_3

Biaxial
 $\alpha = 1.536$
Colorless

$2V \sim 90^\circ$
 $\gamma = 1.568$

Zinc fluoride, ZnF_2

Uniaxial +
 $\omega = 1.501$
Colorless

$\epsilon = 1.526$

Zinc zirconium fluoride, $\text{ZnF}_2 \cdot \text{ZrF}_4$

Cubic
 $n = 1.434$
Colorless.

Zirconium chloride, ZrCl_4

Probably monoclinic
Biaxial
 $\alpha = 1.76$
 $Z\Delta c = 22^\circ$
Colorless

$2V =$ Large
 $\gamma = 1.83$

Zirconium uranium fluoride, $3 \text{ZrF}_4 \cdot \text{UF}_3$

Biaxial
 $n = 1.560$ approximate average
Red
X-ray lines: 4.11, 3.72, 2.06

$2V =$ Large

PART II

X-RAY DIFFRACTION DATA

A. X-ray diffraction patterns for the compounds listed below are included in this section:

BeF₂
 2CsF·BeF₂
 CsF·BeF₂
 3CsF·LaF₃
 2CsF·UF₄
 CsF·UF₄
 2CsF·ZrF₄
 CsF·ZrF₄
 CrF₂
 CrF₃
 CrF₂·ZrF₄
 FeF₂·ZrF₄
 3LiF·CrF₃
 3LiF·NiF₂
 4LiF·UF₄
 3LiF·UF₄
 7LiF·6UF₄
 LiF·4UF₄
 3LiF·ZrF₄
 2LiF·ZrF₄
 3LiF·4ZrF₄
 NiF₂·ZrF₄
 3KF·BeF₂
 KF·BeF₂
 KF·2BeF₂
 3KF·CrF₃
 KF·LaF₃
 KF·NaF·BeF₂
 KF·2NaF·UF₄
 3KF·3NaF·2ZrF₄

3KF·2NaF·5ZrF₄
 KF·NaF·ZrF₄
 2KF·NiF₂
 KF·TeF₄
 7KF·6UF₄
 3KF·2ZrF₄
 α-KF·ZrF₄
 β-KF·ZrF₄
 3RbF·BeF₂
 2RbF·BeF₂
 RbF·BeF₂
 RbF·2BeF₂
 3RbF·CrF₃
 RbF·LaF₃
 RbF·2NaF·BeF₂
 RbF·NaF·UF₄
 3RbF·3NaF·2ZrF₄
 3RbF·UF₄
 2RbF·UF₄
 7RbF·6UF₄
 RbF·UF₄
 2RbF·3UF₄
 RbF·3UF₄
 RbF·6UF₄
 3RbF·ZrF₄
 2RbF·ZrF₄
 5RbF·4ZrF₄
 αRbF·ZrF₄
 βRbF·ZrF₄
 3RbF·3NaF·4ZrF₄

RbF·NaF·2ZrF₄
 RbF·NaF·ZrF₄
 NaF·CeF₃
 NaF·CrF₂
 3NaF·HfF₄
 NaF·HfF₄
 NaF·FeF₂
 NaF·LaF₃
 NaF·2LiF·CrF₃
 NaF·NiF₂
 2NaF·ThF₄
 NaF·UF₃
 α-3NaF·UF₄
 β-3NaF·UF₄
 β-2 2NaF·UF₄
 β-3 2NaF·UF₄
 γ 2NaF·UF₄
 5NaF·3UF₄
 7NaF·6UF₄
 NaF·2UF₄
 3NaF·ZrF₄
 β-1 2NaF·ZrF₄
 β-2 2NaF·ZrF₄
 β-3 2NaF·ZrF₄
 β-4 2NaF·ZrF₄
 γ 2NaF·ZrF₄
 7NaF·6ZrF₄
 3NaF·4ZrF₄
 UF₃·3ZrF₄
 ZnF₂·ZrF₄

Beryllium Fluoride, BeF_2 ⁽¹⁾

$d(\text{\AA})$	I/I_1	Lkl
4.09	70	100
3.21	100	101
2.367	100	110
2.189	100	102
2.154	100	111
1.905	70	201
1.748	50	112
1.606	35	202
1.591	20	103
1.550	30	210
1.484	30	211
1.320	30	203
1.233	15	104
1.208	15	302

Cesium Beryllium Fluoride, $2\text{CsF} \cdot \text{BeF}_2$

$d(\text{\AA})$	I/I_1
5.34	10
4.46	25
4.02	15
3.80	15
3.62	60
3.40	30
3.28	10
3.23	100
3.08	80
2.871	10
2.685	10
2.636	35
2.543	20
2.398	20
2.355	15
2.242	20
2.164	15
2.106	20
2.079	15
2.025	15
2.000	10
1.959	10
1.901	30
1.822	10
1.805	5
1.770	10
1.724	15
1.673	10
1.620	5
1.584	5
1.541	10

Cesium Beryllium Fluoride,
CsF·BeF₂

$\overset{\circ}{d}(\text{\AA})$	I/I_1
5.99	10
5.43	50
4.25	5
3.98	10
3.85	35
3.60	30
3.55	35
3.47	85
3.31	10
3.20	100
3.00	40
2.822	10
2.667	5
2.622	10
2.413	10
2.367	25
2.184	10
2.130	20
2.115	10
1.975	10
1.928	5
1.812	15
1.779	10
1.599	10

Cesium Lanthanum Fluoride,
3CsF·LaF₃

$\overset{\circ}{d}(\text{\AA})$	I/I_1
3.49	100
2.478	35
2.021	60
1.751	20
1.569	12

Cesium Uranium Fluoride
2CsF·UF₄

$\overset{\circ}{d}(\text{\AA})$	I/I_1
6.92	15
6.19	50
4.90	15
4.04	10
3.98	10
3.93	35
3.80	25
3.65	35
3.59	45
3.55	100
3.44	100
3.31	15
3.29	15
3.09	15
3.00	10
2.93	5
2.89	10
2.814	20
2.731	15
2.652	10
2.475	20
2.453	20
2.286	15
2.226	10
2.101	20
2.060	40
2.034	55
1.955	10
1.815	5
1.776	20
1.770	20
1.708	10
1.640	5
1.601	10

Cesium Uranium Fluoride,
CsF·UF₄

$d(\text{\AA})$	I/I_1
8.04	45
7.31	70
5.80	20
5.30	10
5.13	5
4.48	10
4.35	5
4.15	20
4.00	80
3.78	15
3.62	100
3.55	70
3.25	20
3.17	10
2.875	40
2.822	10
2.739	5
2.660	20
2.615	5
2.410	35
2.292	10
2.244	10
2.189	10
2.111	5
2.069	35
2.025	25
2.000	30
1.916	10
1.890	5
1.805	60
1.757	5
1.679	5
1.654	10
1.609	10
1.538	5
1.532	5
1.520	5
1.485	5

Cesium Zirconium Fluoride,
2CsF·ZrF₄

$d(\text{\AA})$	I/I_1
4.11	35
3.88	5
3.73	100
3.54	10
3.34	5
3.20	40
2.96	10
2.771	10
2.687	10
2.529	5
2.501	10
2.430	40
2.286	20
2.140	5
2.056	5
1.932	20
1.857	20
1.779	5
1.773	5
1.667	10
1.609	10
1.601	10
1.480	10

Cesium Zirconium Fluoride
CsF·ZrF₄

<u>d(Å)</u>	<u>I/I₁</u>
6.76	35
6.30	15
5.87	10
5.45	10
5.07	15
4.80	10
4.37	20
4.33	20
4.00	15
3.91	25
3.85	15
3.73	100
3.62	85
3.42	50
3.26	85
3.12	40
2.593	15
2.333	10
2.264	15
2.222	25
2.164	10
2.079	15
1.932	15
1.879	15
1.658	10
1.543	15

Chromium(II) Fluoride
CrF₂

<u>d(Å)</u>	<u>I/I₁</u>
3.690	20
3.56	5
3.35	50
3.28	25
3.10	10
2.97	100
2.805	30
2.660	5
2.508	15
2.398	10
2.355	10
2.322	5
2.074	10
1.884	15
1.843	10
1.763	15
1.743	10
1.665	10
1.594	10

Chromium(III) Fluoride
CrF₃

<u>d(Å)</u>	<u>I/I₁</u>
4.00	30
3.62	100
2.91	5
2.885	5
2.622	25
2.501	10
2.410	10
2.169	25
2.004	5
1.829	10
1.809	20
1.649	30
1.622	5
1.586	10
1.543	10

Chromium Zirconium Fluoride,
 $\text{CrF}_2 \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
4.72	10
4.55	30
4.41	10
4.09	100
4.00	45
3.88	5
2.866	25
2.275	15
2.065	65
1.999	25
1.829	25
1.799	15
1.667	10

Lithium Chromium Fluoride,
 $3\text{LiF} \cdot \text{CrF}_3$

$d(\text{\AA})$	I/I_1
4.29	45
4.16	100
3.45	35
2.67	30
2.212	25
2.176	80
2.140	25
2.092	20
2.008	10
1.736	10
1.730	25
1.712	35

Iron Zirconium Fluoride
 $\text{FeF}_2 \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
4.95	10
4.65	40
4.48	45
4.35	8
4.04	100
3.16	15
2.857	45
2.436	8
2.237	15
2.016	50
1.997	25
1.805	65
1.649	25
1.489	15
1.426	10
1.412	15

Lithium Nickel Fluoride
 $3\text{LiF} \cdot \text{NiF}_2$

$d(\text{\AA})$	I/I_1
4.81	95
3.06	8
2.508	95
2.074	100
2.016	95
1.599	45
1.470	45
1.426	10
1.405	10

Lithium Uranium Fluoride
4LiF·UF₄

$d(\text{\AA})$	I/I_1
5.67	20
5.46	25
5.13	70
4.93	100
4.55	45
4.44	100
4.23	7
3.82	40
3.55	30
3.03	50
2.89	25
2.866	30
2.747	50
2.468	40
2.398	20
2.221	40
2.167	75
2.074	20
2.025	20
1.872	20
1.836	25

Lithium Uranium Fluoride
3LiF·UF₄ (2)

$d(\text{\AA})$	I/I_1
4.98	20
4.80	15
4.41	100
4.34	100
3.98	15
3.91	8
3.60	80
3.40	10
3.14	25
3.07	50
2.84	80
2.771	30
2.529	35
2.169	15
2.083	75
2.055	35
1.943	50
1.913	25
1.861	30
1.751	25
1.723	25
1.685	25
1.662	8
1.646	20
1.599	8

Lithium Uranium Fluoride
7LiF·6UF₄

<u>d (Å)</u>	<u>I/I₁</u>
6.61	6
5.97	20
5.82	15
5.24	90
5.15	10
4.65	10
4.37	13
3.95	55
3.85	13
3.68	20
3.49	75
3.33	90
3.15	70
3.07	10
2.99	95
2.771	30
2.707	30
2.542	25
2.350	13
2.286	25
2.264	13
2.184	10
2.097	30
2.060	30
2.047	75
1.993	25
1.972	20
1.947	25
1.924	15
1.909	30
1.854	45
1.825	20
1.773	20
1.757	25
1.709	15
1.680	15
1.625	15
1.579	25
1.562	8

Lithium Uranium Fluoride
LiF·4UF₄

<u>d (Å)</u>	<u>I/I₁</u>
7.02	8
6.33	12
6.07	5
5.73	25
4.98	8
4.70	25
4.25	90
3.88	20
3.78	100
3.52	90
3.16	8
3.13	8
3.06	12
2.84	40
2.771	55
2.542	8
2.350	10
2.310	10
2.226	8
2.000	10
2.088	35
2.016	60
1.991	50
1.888	20
1.819	8
1.767	25

Lithium Zirconium Fluoride
(low temperature form)
 $3\text{LiF} \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
5.49	55
5.40	35
4.88	50
3.67	25
3.43	5
2.91	15
2.79	8
2.67	15
2.40	5
2.07	100
1.94	20
1.82	25
1.80	12
1.78	12
1.65	5
1.59	5
1.57	5

Lithium Zirconium Fluoride
 $2\text{LiF} \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
5.14	10
4.75	10
4.62	25
4.29	100
3.15	100
2.75	10
2.49	15
2.42	10
2.38	10
2.26	7
2.19	60
2.15	20
2.05	20
1.95	25
1.70	30
1.63	45
1.58	10
1.54	10

Lithium Zirconium Fluoride
(high temperature form)
 $3\text{LiF} \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
7.2	15
6.42	15
5.68	15
4.58	100
3.75	15
3.68	12
3.43	15
3.24	30
3.15	60
2.84	40
2.63	20
2.535	10
2.361	15
2.20	10
2.047	65
1.847	20

Lithium Zirconium Fluoride
3LiF·4ZrF₄

$d(\text{\AA})$	I/I_1
6.11	25
5.24	35
4.90	15
4.21	30
4.00	10
3.90	95
3.77	20
3.69	5
3.33	60
3.29	20
3.26	20
3.16	100
2.615	15
2.303	10
2.248	10
2.227	5
2.194	85
2.159	15
2.043	12
2.130	35
1.947	35
1.912	20
1.883	10
1.721	10

Potassium Beryllium Fluoride
3KF·BeF₂

$d(\text{\AA})$	I/I_1
3.42	5
3.30	7
3.07	25
2.98	75
2.81	10
2.64	30
2.54	35
2.51	15
2.39	100
2.27	70
2.04	5
1.96	5
1.85	12
1.78	12
1.73	10
1.72	10
1.69	7
1.60	5
1.56	5
1.54	5

Nickel Zirconium Fluoride
NiF₂·ZrF₄

$d(\text{\AA})$	I/I_1
4.88	15
4.50	5
3.91	100
2.805	50
2.763	10
2.367	15
2.174	5
1.964	50
1.767	55
1.745	15
1.622	10
1.596	10

Potassium Beryllium Fluoride
KF·BeF₂

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
6.65	15
5.99	60
3.69	5
3.58	10
3.33	90
3.23	35
3.01	100
2.92	5
2.734	15
2.636	20
2.542	5
2.442	5
2.410	5
2.292	15
2.220	7
2.190	5
2.010	35
1.979	25
1.745	7
1.641	10

Potassium Chromium(III) Fluoride
3KF·CrF₃

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
4.95	35
4.26	15
3.35	35
3.03	100
2.475	25
2.154	20
2.135	55
1.743	15
1.516	15

Potassium Beryllium Fluoride
KF·2BeF₂

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
5.99	10
3.66	15
3.31	60
3.00	100
2.65	5
2.55	5
2.44	5
2.39	15
2.37	5
2.29	15
2.21	15
2.14	15
2.08	5
2.01	5
2.00	5
1.83	5
1.78	10
1.60	5

Potassium Lanthanum Fluoride
KF·LaF₃

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
7.77	100
5.61	70
4.90	35
3.32	40
3.26	60
3.15	65
2.747	100
2.209	40
1.951	25
1.920	20
1.894	12
1.883	30
1.857	65
1.662	20
1.641	5
1.577	20

Potassium Nickel Fluoride⁽⁶⁾
2KF·NiF₂

<u>d (Å)</u>	<u>I/I₁</u>
6.51	100
5.85	45
3.83	10
2.94	55
2.830	35
2.344	5
2.212	10
2.173	100
2.135	15
1.999	55
1.909	15
1.805	10
1.730	30
1.654	10
1.633	35
1.594	10
1.474	20

Potassium Sodium Beryllium Fluoride
KF·NaF·BeF₂

<u>d (Å)</u>	<u>I/I₁</u>
7.08	5
3.85	25
3.17	15
3.08	30
2.866	60
2.786	100
2.675	10
2.626	60
2.593	10
2.528	15
2.410	10
2.367	100
2.287	70
2.212	15
2.189	10
2.159	10
2.125	5
1.995	60
1.967	10
1.819	5
1.806	5
1.777	25
1.691	10
1.620	10
1.605	15

Potassium Sodium Uranium Fluoride
KF·2NaF·UF₄

<u>d (Å)</u>	<u>I/I₁</u>
8.64	25
7.80	80
6.00	15
5.42	65
4.93	30
4.44	90
3.51	40
3.46	25
3.16	100
3.13	100
2.90	35
2.830	5
2.710	20
2.593	10
2.557	20
2.462	20
2.443	5
2.344	20
2.321	5
2.222	80
2.189	5
2.156	5
2.074	5
2.047	10
1.995	25
1.977	25
1.947	20
1.872	20
1.833	20
1.809	65
1.776	5
1.754	15
1.727	5
1.654	25
1.606	15
1.579	10
1.560	15

Potassium Sodium Zirconium
Fluoride, $3\text{KF} \cdot 3\text{NaF} \cdot 2\text{ZrF}_4$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
6.11	15
4.90	100
4.82	25
4.55	15
4.27	55
4.09	75
3.78	12
3.40	20
3.28	20
2.99	20
2.97	90
2.72	12
2.682	12
2.585	5
2.455	25
2.417	20
2.368	12
2.270	25
2.226	50
2.135	40
2.051	50
1.931	15
1.822	40
1.748	20
1.721	25

Potassium Sodium Zirconium
Fluoride, $3\text{KF} \cdot 2\text{NaF} \cdot 5\text{ZrF}_4$

$d(\text{\AA})$	I/I_1
8.51	100
7.70	100
6.20	3
5.57	5
5.15	8
5.01	20
4.77	8
4.65	35
4.29	40
3.86	100
3.75	15
3.50	15
3.40	50
3.23	5
3.17	60
3.09	35
2.87	5
2.80	10
2.58	5
2.47	5
2.39	8
2.33	8
2.19	5
2.16	8
2.14	50
2.09	8
2.06	8
1.95	30
1.94	90
1.91	10
1.89	10
1.88	15
1.84	7
1.81	7
1.76	8
1.70	13

Potassium Sodium Zirconium
Fluoride, $\text{KF} \cdot \text{NaF} \cdot \text{ZrF}_4$

$\overset{\text{O}}{\text{d(A)}}$	I/I_1
5.99	10
5.37	50
4.98	15
4.85	60
4.50	50
4.41	5
4.25	30
4.09	65
3.69	30
3.60	12
3.52	5
3.34	100
3.26	45
3.18	40
3.12	12
3.07	12
3.01	40
2.747	5
2.690	25
2.556	20
2.489	25
2.405	20
2.258	20
2.154	16
2.215	20
2.050	35
1.947	20
1.928	12
1.886	12
1.792	15
1.743	20
1.723	15
1.694	5
1.651	25

Potassium Tellurium Fluoride
 $\text{KF} \cdot \text{TeF}_4 \cdot \text{H}_2\text{O}$

d(A)	I/I_1
5.64	100
4.61	60
4.27	100
3.95	10
3.575	75
3.170	15
2.910	25
2.805	50
2.303	25
2.134	10
2.034	10
1.963	45
1.872	20
1.812	10
1.779	10
1.742	15
1.641	5
1.606	10

Potassium Uranium Fluoride (4b)
7KF·6UF₄

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
8.11	50
7.50	20
5.54	15
4.93	10
4.82	60
4.46	50
4.35	30
4.17	10
4.06	15
3.78	55
3.58	20
3.44	100
3.29	15
3.12	10
2.97	65
2.885	15
2.858	20
2.710	15
2.550	10
2.515	10
2.409	10
2.368	10
2.333	20
2.321	25
2.298	25
2.243	15
2.200	30
2.140	15
2.111	70
2.096	80
2.047	10
2.030	10
1.995	25
1.987	40
1.983	40
1.959	10
1.913	10
1.896	10
1.861	10
1.840	10
1.802	45
1.793	70
1.789	70
1.757	10
1.730	10

$\overset{\text{O}}{d(\text{\AA})}$ I/I_1

1.715	30
1.654	10
1.606	10
1.589	10
1.582	10
1.553	10

Potassium Zirconium Fluoride
3KF·2ZrF₄

$\overset{\text{O}}{d(\text{\AA})}$ I/I_1

7.37	10
6.56	20
5.95	75
5.54	70
5.09	15
4.95	25
4.90	20
4.39	40
3.97	100
3.83	10
3.71	20
3.66	20
3.56	15
3.45	15
3.33	100
3.31	85
3.11	75
2.571	10
2.550	15
2.270	15
2.214	25
2.200	65
2.111	10
1.979	100
1.883	10
1.842	25
1.739	10
1.705	20
1.673	20

Potassium Zirconium Fluoride
 α -KF·ZrF₄

$d(\text{\AA})$	I/I_1
5.83	60
4.89	35
4.40	80
4.29	20
4.07	5
3.86	100
3.08	20
2.90	10
2.52	5
2.475	15
2.232	5
2.200	20
2.140	15
2.088	10
2.043	5
2.016	10
1.912	5
1.850	10
1.779	5

Potassium Zirconium Fluoride
 β -KF·ZrF₄

$d(\text{\AA})$	I/I_1
8.26	7
6.97	50
6.32	100
5.50	15
5.31	30
3.93	15
3.49	40
3.36	35
3.29	60
3.15	100
2.763	7
2.731	10
2.392	15
2.332	15
2.179	12
2.120	12
2.106	40
2.065	15
1.967	10
1.916	60
1.865	15
1.843	35
1.748	15
1.665	5
1.579	70

Rubidium Beryllium Fluoride
3RbF·BeF₂

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
3.83	10
3.55	10
3.45	35
3.21	10
3.11	10
2.95	60
2.755	10
2.655	5
2.629	5
2.488	55
2.373	5
2.125	25
2.047	15
1.987	5
1.920	10
1.809	15
1.799	15
1.688	40
1.577	35
1.531	5
1.425	100
1.421	100
1.328	10

Rubidium Beryllium Fluoride
2RbF·BeF₂

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
5.10	10
4.25	20
3.98	5
3.82	15
3.59	10
3.45	50
3.40	25
3.26	30
3.22	10
3.11	15
3.07	100
2.95	100
2.822	15
2.747	10
2.691	20
2.592	5
2.556	90
2.482	60
2.423	70
2.350	5
2.338	5
2.275	25
2.242	15
2.125	25
2.097	5
2.065	5
2.047	50
1.975	10
1.928	25
1.897	30
1.868	25
1.799	20
1.730	35
1.699	15
1.641	10
1.599	5
1.472	20
1.468	10

Rubidium Beryllium Fluoride
RbF·BeF₂

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
6.28	5
5.24	20
4.70	5
4.49	5
4.24	20
4.17	10
3.85	20
3.74	45
3.62	10
3.58	5
3.46	100
3.38	100
3.26	10
3.18	10
3.12	100
3.03	10
2.96	15
2.87	20
2.739	25
2.564	5
2.521	10
2.496	10
2.482	5
2.430	10
2.394	10
2.367	5
2.332	15
2.300	35
2.275	45
2.104	15
2.076	100
2.052	35
1.947	10
1.920	10
1.883	10
1.861	10
1.825	15
1.802	10
1.735	15
1.723	15
1.699	30
1.680	10
1.630	10
1.614	10
1.578	10
1.557	35
1.552	25

Rubidium Beryllium Fluoride
RbF·2BeF₂

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
6.16	70
3.39	40
3.31	20
3.10	100
2.715	5
2.475	35
2.410	15
2.327	10
2.201	5
2.149	20
1.876	5
1.852	10
1.819	15
1.552	15

Rubidium Chromium Fluoride
3RbF·CrF₃

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
3.47	12
3.16	100
3.13	55
3.11	55
2.98	12
2.57	15
2.468	12
2.350	5
2.315	10
2.264	20
2.208	40
2.149	10
2.088	10
1.829	10
1.813	10
1.805	25
1.625	10
1.582	25
1.582	25

Rubidium Lanthanum Fluoride
RbF·LaF₃

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
8.11	25
5.07	15
4.04	8
3.43	100
2.48	25
2.25	40
1.97	15
1.93	15
1.90	40
1.87	12
1.71	15
1.68	15
1.46	8

Rubidium Sodium Uranium Fluoride
RbF·NaF·UF₄

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
8.12	100
7.20	10
6.48	30
5.47	60
5.02	10
4.55	55
3.77	45
3.26	80
3.15	60
2.94	10
2.862	5
2.723	10
2.588	15
2.508	20
2.430	15
2.264	60
2.211	5
2.106	10
2.051	10
2.034	75
1.995	10
1.920	10
1.905	30
1.838	40
1.815	15
1.799	10
1.773	7
1.701	25
1.625	25
1.574	5
1.555	10

Rubidium Sodium Beryllium
Fluoride, RbF·2NaF·BeF₂

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
4.60	25
4.15	85
3.75	40
2.99	100
2.875	100
2.767	70
2.618	20
2.494	100
2.362	60
2.295	30
2.232	10
2.189	10
2.074	85
1.987	15
1.939	5
1.883	30
1.872	10
1.825	25
1.751	20
1.682	30
1.657	25
1.586	15
1.569	10
1.495	30

Rubidium Sodium Zirconium
Fluoride, $3\text{RbF} \cdot 3\text{NaF} \cdot 2\text{ZrF}_4 (2)$

$d(\text{\AA})$	I/I_1
4.32	55
4.15	30
3.57	20
3.33	20
3.22	55
3.09	15
3.00	100
2.747	10
2.481	10
2.450	10
2.281	30
2.164	25
2.125	9
2.079	30
1.920	15
1.868	30
1.767	15
1.742	25
1.500	25

Rubidium Uranium Fluoride
 $3\text{RbF} \cdot \text{UF}_4$

$d(\text{\AA})$	I/I_1
8.43	7
6.03	10
5.56	35
5.13	5
4.83	10
3.80	10
3.72	10
3.58	10
3.48	15
3.40	100
3.24	20
3.01	7
2.89	15
2.593	7
2.521	10
2.482	7
2.398	30
2.275	5
2.194	10
2.140	7
2.101	15
1.959	60
1.912	5
1.897	5
1.844	10
1.694	15
1.623	7

Rubidium Uranium Fluoride
(low temperature form)
 $2\text{RbF} \cdot \text{UF}_4$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
6.03	100
4.75	15
3.49	100
3.23	25
3.17	10
3.02	20
2.814	10
2.367	20
2.281	10
2.184	45
2.008	65
1.963	10
1.947	35
1.909	5
1.740	15
1.699	15
1.673	15
1.635	25
1.584	5
1.538	5
1.511	5
1.476	10

Rubidium Uranium Fluoride
 $7\text{RbF} \cdot 6\text{UF}_4$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
8.35	15
4.98	15
4.57	15
4.46	7
4.17	5
3.85	10
3.68	5
3.58	20
3.51	100
3.05	45
2.259	7
2.169	25
2.140	50
2.030	7
1.890	15
1.854	15
1.835	45
1.786	7
1.751	20
1.522	15

Rubidium Uranium Fluoride
 $\text{RbF} \cdot \text{UF}_4$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
8.26	5
7.56	10
6.86	100
4.44	15
4.02	15
3.96	10
3.85	5
3.79	5
3.56	10
3.46	50
3.43	100
3.25	5
3.04	12
2.630	5
2.607	10
2.527	10
2.315	5
2.286	20
2.201	10
2.164	7
2.130	7
2.008	5
1.987	30
1.916	5
1.901	10
1.865	5
1.850	5
1.829	5
1.733	5
1.714	25
1.579	5
1.518	5

Rubidium Uranium Fluoride
2RbF · 3UF₄

<u>d(A)</u>	<u>I/I₁</u>
6.39	12
5.80	45
5.04	7
4.18	7
3.86	40
3.50	100
3.22	15
3.07	5
2.780	10
2.614	15
2.417	10
2.361	10
2.259	25
2.184	30
2.038	60
1.943	10
1.935	5
1.843	10
1.805	10
1.773	7

Rubidium Uranium Fluoride
RbF · 3UF₄

<u>d(A)</u>	<u>I/I₁</u>
7.97	60
7.63	10
7.31	15
6.71	10
6.32	5
5.80	5
5.57	10
5.50	20
5.38	10
5.01	10
4.55	30
4.41	15
4.31	5
4.23	25
4.15	15
4.09	5
4.04	10
3.99	20
3.88	25
3.73	40
3.66	55

⁰ <u>d(A)</u>	<u>I/I₁</u>
3.59	15
3.52	100
3.43	10
3.36	80
3.34	35
3.24	60
3.10	35
3.00	5
2.98	5
2.90	40
2.848	10
2.736	10
2.706	20
2.667	10
2.629	20
2.571	15
2.501	10
2.469	10
2.433	5
2.404	15
2.341	15
2.315	5
2.247	15
2.237	15
2.216	40
2.159	20
2.111	5
2.088	20
2.070	10
2.043	15
2.034	20
2.025	80
2.002	100
1.951	60
1.903	10
1.883	10
1.870	40
1.847	15
1.831	30
1.809	10
1.789	10
1.757	25
1.720	35
1.659	25
1.614	10
1.594	20
1.589	15
1.577	5
1.564	10
1.550	20

Rubidium Uranium Fluoride
RbF·6UF₄

$d(\text{\AA})$	I/I_1
7.14	15
6.53	20
4.82	10
4.56	25
4.35	30
4.13	75
3.93	20
3.85	25
3.68	10
3.55	50
3.47	100
3.30	10
3.22	10
3.11	10
3.05	5
2.98	60
2.90	25
2.747	10
2.686	20
2.410	15
2.367	5
2.270	15
2.172	20
2.049	75
2.030	10
2.006	20
1.957	45
1.833	40
1.763	20
1.724	5
1.688	15
1.641	10
1.630	10
1.620	5
1.606	5

Rubidium Zirconium Fluoride
3RbF·ZrF₄

simple cubic $a_0 = 3.288 \text{ \AA}$

$d(\text{\AA})$	I/I_1
3.290	100
2.326	60
1.900	100
1.646	20

Rubidium Zirconium Fluoride
2RbF·ZrF₄
(low temperature form)

5.350	10
4.835	8
3.590	100
3.080	34
2.414	5
2.338	40
2.199	20
1.861	15
1.789	15
1.569	12
1.422	8

Rubidium Zirconium Fluoride
 $5\text{RbF} \cdot 4\text{ZrF}_4$

$d(\text{\AA})$	I/I_1
5.87	10
5.61	10
5.04	10
4.77	15
4.50	12
4.29	65
3.98	25
3.82	30
3.78	15
3.72	15
3.63	30
3.59	95
3.52	8
3.44	100
3.42	100
3.36	100
3.29	100
3.05	12
2.60	25
2.508	30
2.386	12
2.350	75
2.281	10
2.275	12
2.260	12
2.253	12
2.245	8
2.226	12
2.152	45
2.067	12
2.027	12
1.959	30
1.932	30
1.897	15
1.868	20
1.833	20
1.770	30
1.763	30
1.679	12

Rubidium Zirconium Fluoride
 $\alpha\text{-RbF} \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
7.13	40
5.95	20
4.28	10
4.02	10
3.83	80
3.69	25
3.59	5
3.45	100
3.42	100
3.34	100
3.07	15
3.01	10
2.699	10
2.622	10
2.574	20
2.550	7
2.450	10
2.423	25
2.327	14
2.226	10
2.184	10
2.149	10
2.118	10
2.056	25
1.991	10
1.957	25
1.928	10
1.905	20
1.868	15
1.812	15
1.782	10
1.763	10
1.742	10
1.670	15
1.611	10
1.547	10
1.502	15

Rubidium Zirconium Fluoride
 β -RbF·ZrF₄

$d(\text{\AA})$	I/I_1	$d(\text{\AA})$	I/I_1
7.37	12	2.191	30
6.66	40	2.116	40
6.32	5	2.074	10
5.53	5	2.034	5
5.17	5	1.997	30
5.01	20	1.989	50
4.67	5	1.935	50
4.54	5	1.929	50
4.46	5	1.926	55
4.35	12	1.903	30
3.99	12	1.894	5
3.88	5	1.872	12
3.77	30	1.857	10
3.72	35	1.836	10
3.69	40	1.773	5
3.61	40	1.757	5
3.42	100	1.751	5
3.36	100	1.742	5
3.325	100	1.731	15
3.090	10	1.728	15
3.060	15	1.719	24
2.960	5	1.716	15
2.900	5	1.709	15
2.822	5	1.699	10
2.788	40	1.694	10
2.767	45	1.679	20
2.678	5	1.662	5
2.614	5	1.654	20
2.564	5		
2.514	8		
2.501	8		
2.482	5		
2.455	5		
2.433	5		
2.423	5		
2.398	5		
2.380	10		
2.355	10		
2.344	10		
2.309	5		
2.292	8		
2.253	5		
2.240	12		
2.211	15		
2.206	15		

Rubidium Sodium Zirconium
Fluoride, $3\text{RbF} \cdot 3\text{NaF} \cdot 4\text{ZrF}_4$

$d(\text{\AA})$	I/I_1
6.77	5
6.11	15
5.72	15
5.37	30
4.67	9
4.21	35
4.11	10
3.98	15
3.82	20
3.72	30
3.56	5
3.50	10
3.44	100
3.31	8
3.22	30
3.17	65
3.11	100
3.07	5
3.01	20
2.95	5
2.571	10
2.482	8
2.356	8
2.243	8
2.164	10
2.111	15
2.088	15
2.060	35
2.025	30
2.004	8
1.976	8
1.947	30
1.909	20
1.861	85
1.812	5
1.727	10
1.638	10
1.591	10

Rubidium Sodium Zirconium
Fluoride, $\text{RbF} \cdot \text{NaF} \cdot 2\text{ZrF}_4$

$d(\text{\AA})$	I/I_1
7.43	5
6.71	5
6.54	5
5.91	40
4.55	20
4.41	5
4.13	50
3.90	8
3.71	60
3.52	45
3.40	8
3.35	100
3.29	12
3.23	10
3.13	12
2.826	20
2.481	5
2.430	5
2.392	5
2.380	5
2.344	5
2.286	5
2.237	5
2.194	10
2.159	20
2.142	10
2.083	5
2.060	10
1.983	8
1.963	12
1.943	15
1.935	25
1.920	5
1.854	8
1.836	8
1.757	40
1.754	45
1.694	8
1.676	40
1.670	30

Rubidium Sodium Fluoride
RbF·NaF·ZrF₄

$\bar{d}(\text{\AA})$	I/I_1
5.21	10
4.82	5
4.68	40
4.21	45
3.75	15
3.65	5
3.59	10
3.39	65
3.34	10
3.29	20
3.24	35
2.571	10
2.514	8
2.350	15
2.332	30
2.321	30
2.152	100
2.094	100
1.886	10
1.763	20
1.614	8

Sodium Cerium Fluoride
NaF·CeF₃

$\bar{d}(\text{\AA})$	I/I_1
5.95	15
5.35	60
3.43	40
3.09	90
2.57	100
2.411	10
2.392	15
2.179	35
2.097	5
2.016	5
1.967	25
1.894	10
1.843	10
1.815	10
1.777	90
1.612	10
1.538	15
1.375	15

Rubidium Uranium Fluoride
RbF·UF₃

$\bar{d}(\text{\AA})$	I/I_1
8.12	30
5.07	15
4.04	7
3.43	100
2.485	25
2.253	40
1.968	15
1.932	12
1.898	40
1.869	40
1.715	15
1.682	15
1.460	8

Sodium Chromium (II) Fluoride
NaF·CrF₂

$\bar{d}(\text{\AA})$	I/I_1
5.15	5
4.63	15
4.49	10
3.95	15
3.01	100
2.593	10
2.368	10
2.189	15
2.039	25
1.975	20

Sodium Hafnium Fluoride
3NaF·HfF₄

<u>d(Å)</u>	<u>I/I₁</u>
5.27	55
4.27	90
3.77	50
3.07	100
2.94	40
1.967	30
1.883	10
1.872	75
1.770	15
1.603	50
1.586	5

Sodium Hafnium Fluoride
NaF·HfF₄

<u>d(Å)</u>	<u>I/I₁</u>
7.37	30
5.61	100
5.37	80
5.04	15
4.37	30
4.17	20
4.05	45
3.98	60
3.87	100
3.69	10
3.45	15
3.35	20
3.31	15
3.26	15
3.13	85
3.03	20
2.85	20
2.82	20
2.75	15
2.71	40
2.62	10
2.51	35
2.49	15
2.28	40
2.21	40
2.03	10
2.02	10
1.99	15
1.95	15
1.91	60
1.86	35
1.84	10
1.81	10
1.78	35
1.73	15
1.71	40
1.66	25
1.65	55
1.63	65
1.61	5
1.58	10
1.56	15
1.55	15

Sodium Iron (II) Fluoride
NaF·FeF₂

$\overset{\circ}{d}(\text{\AA})$	I/I_1
4.35	25
3.92	90
3.08	15
2.83	30
2.78	50
2.731	12
2.462	15
2.174	45
1.964	100
1.783	35
1.757	20
1.739	12

Sodium Lithium Chromium Fluoride
NaF·2LiF·CrF₃

$\overset{\circ}{d}(\text{\AA})$	I/I_1
4.36	100
4.17	20
3.17	10
3.08	60
2.76	15
2.68	15
2.629	15
2.515	20
2.416	20
2.327	10
2.247	30
2.216	10
2.176	20
2.097	10
2.012	5
1.995	30
1.947	40
1.708	20

Sodium Lanthanum Fluoride (4a)
NaF·LaF₃

$\overset{\circ}{d}(\text{\AA})$	I/I_1
5.37	65
3.11	100
2.09	100
2.69	15
2.405	20
2.194	90
2.021	15
1.913	15
1.783	80
1.627	15
1.545	12
1.485	10
1.383	20

Sodium Nickel Fluoride
NaF·NiF₂

<u>d(Å)</u>	<u>I/I₁</u>
4.25	10
3.85	100
3.45	8
3.33	5
3.05	5
3.01	10
2.764	35
2.723	50
2.682	20
2.398	10
2.327	10
2.309	25
2.130	15
2.070	10
2.034	25
1.924	100
1.796	5
1.757	20
1.742	35
1.720	30
1.697	10
1.586	20
1.579	20
1.557	40

Sodium Thorium Fluoride (4a)
2NaF·ThF₄

<u>d(Å)</u>	<u>I/I₁</u>
6.22	10
5.72	45
5.38	10
5.17	100
4.53	10
4.11	20
3.83	5
3.69	5
3.65	5
3.40	10
3.31	15
3.07	35
2.99	70
2.863	20
2.590	55
2.442	5
2.374	10
2.352	20
2.197	40
2.056	5
1.987	5
1.955	15
1.928	15
1.909	10
1.793	10
1.742	55
1.724	20
1.705	5
1.609	5
1.572	5

Sodium Uranium (III) Fluoride
 $\text{NaF} \cdot \text{UF}_3$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
5.34	30
3.09	100
2.392	15
2.179	55
2.016	50
1.898	10
1.779	75
1.614	10
1.541	10

Sodium Uranium Fluoride (3)
 $\alpha \text{ } 3\text{NaF} \cdot \text{UF}_4$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
5.47	35
4.87	100
3.85	50
3.15	75
3.03	30
2.721	30
2.435	30
2.378	25
2.224	30
2.022	15
1.926	45
1.815	25
1.791	30
1.722	35
1.642	30
1.574	15
1.511	15
1.496	15
1.457	15

Sodium Uranium Fluoride (3)
 $\beta \text{ } 3\text{NaF} \cdot \text{UF}_4$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
6.28	45
5.15	100
3.98	60
3.65	10
3.29	10
2.97	100
2.578	25
2.206	10
2.164	30
2.102	80
1.991	20
1.943	15
1.897	5
1.857	15
1.819	10
1.751	10
1.718	85
1.552	25
1.506	10
1.485	15

Sodium Uranium Fluoride (2, 3, 4a)
 $\beta \text{ } 2\text{ } 2\text{NaF} \cdot \text{UF}_4$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
5.12	100
3.72	10
3.02	85
2.97	40
2.578	35
2.327	55
2.121	90
1.947	35
1.869	15
1.754	15
1.730	100
1.583	15
1.562	25

Sodium Uranium Fluoride (3)
 β -3 $2\text{NaF} \cdot \text{UF}_4$

<u>d (Å)</u>	<u>I/I₁</u>	<u>hkl</u>
7.25	100	001
5.31	20	100
4.28	75	101
3.06	35	110
2.99	60	102
2.817	10	111
2.644	5	200
2.488	15	201
2.410	20	003
2.338	5	112
2.194	10	103
2.135	35	202
1.999	5	210
1.928	15	211
1.890	15	113
1.809	20	004
1.783	5	203
1.760	15	300
1.748	25	212
1.712	15	104
1.555	10	114
1.538	5	213
1.527	5	220
1.491	5	221, 204
1.436	5	311
1.422	5	303
1.394	15	105
1.358	5	312
1.340	5	214

Sodium Uranium Fluoride (2,3)
 γ $2\text{NaF} \cdot \text{UF}_4$

<u>d (Å)</u>	<u>I/I₁</u>
5.79	50
4.92	100
3.78	40
3.24	50
3.17	70
2.91	20
2.831	40
2.767	30
2.501	20
2.235	50
2.173	50
2.151	50
2.003	50
1.967	100
1.947	20
1.896	20
1.860	30
1.826	20
1.696	10
1.669	80

Sodium Uranium Fluoride (4c,5)
 $5\text{NaF} \cdot 3\text{UF}_4$

$d(\text{\AA})$	I/I_1
3.19	100
2.777	30
1.964	65
1.684	65
1.609	15
1.396	15
1.282	-
1.248	-
1.144	-

Sodium Uranium Fluoride (4d,5)
 $7\text{NaF} \cdot 6\text{UF}_4$

$d(\text{\AA})$	I/I_1
7.76	40
5.34	20
4.55	50
4.32	70
4.25	55
3.87	10
3.68	25
3.43	10
3.33	85
3.25	100
3.03	20
2.97	20
2.863	50
2.786	50
2.595	15
2.585	30
2.437	10
2.342	10
2.177	35
2.114	25
2.073	10
2.047	10
2.041	30
1.909	15
1.731	40
1.773	45
1.664	10

Sodium Uranium Fluoride
NaF·2UF₄

<u>d (Å)</u>	<u>I/I₁</u>	<u>d (Å)</u>	<u>I/I₁</u>
7.80	8	2.449	8
6.61	8	2.411	8
6.19	20	2.355	10
6.03	20	2.290	10
5.61	100	2.250	8
5.47	25	2.211	8
5.21	12	2.184	8
4.98	10	2.152	8
4.92	10	2.144	8
4.80	8	2.137	8
4.65	25	2.128	25
4.33	35	2.090	8
4.09	10	2.065	30
4.04	15	2.034	15
3.91	15	2.010	10
3.80	8	1.983	15
3.69	50	1.947	15
3.60	15	1.939	20
3.51	15	1.931	30
3.43	20	1.912	35
3.42	20	1.865	10
3.41	20	1.840	8
3.30	45	1.817	25
3.26	70	1.792	8
3.15	20	1.790	8
3.12	8	1.754	10
3.08	65	1.742	10
2.98	8	1.730	20
2.90	8	1.720	15
2.87	10	1.643	15
2.813	45	1.638	10
2.747	8	1.586	15
2.731	8	1.584	10
2.675	8	1.576	15
2.622	8	1.572	15
2.600	8	1.554	20

Sodium Zirconium Fluoride
3NaF·ZrF₄ (3)

$d(\text{\AA})$	I/I_1
5.25	35
4.75	75
3.75	20
3.06	100
2.93	10
2.32	10
1.97	5
1.88	20
1.87	35
1.77	5
1.60	15
1.59	5
1.46	5

Sodium Zirconium Fluoride
 β -2 2NaF·ZrF₄ (3)

$d(\text{\AA})$	I/I_1
5.72	20
5.47	80
5.38	50
3.78	80
3.31	20
3.11	100
2.675	20
2.410	20
2.216	20
2.043	20
1.912	100
1.897	80
1.793	20
1.645	20
1.617	50
1.557	10

Sodium Zirconium Fluoride
 β -1 2NaF·ZrF₄ (3)

$d(\text{\AA})$	I/I_1
5.45	10
5.15	55
4.73	25
4.06	15
3.83	5
3.72	40
3.48	15
3.43	5
3.15	5
3.09	100
2.839	5
2.682	10
2.593	5
2.327	10
2.237	5
2.206	10
2.169	5
2.088	10
2.038	15
1.995	10
1.951	6
1.890	100
1.847	5
1.812	5
1.776	10
1.711	5
1.688	5
1.630	5
1.611	45

Sodium Zirconium Fluoride
 β -3 2NaF·ZrF₄ (3)

$d(\text{\AA})$	I/I_1
5.12	100
4.80	10
4.55	100
4.00	5
3.89	10
3.60	90
3.24	25
3.12	10
3.04	10
2.95	40
2.893	100
2.557	10
2.550	10
2.475	40
2.275	30
2.221	30
2.085	10
1.894	100
1.799	30
1.708	60
1.608	6
1.543	20

Sodium Zirconium Fluoride
 β -4 $2\text{NaF} \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
7.97	35
5.54	15
5.12	80
4.88	65
4.48	15
4.33	20
4.00	70
3.83	70
3.25	100
3.12	50
3.04	40
2.89	15
2.759	25
2.666	20
2.564	20
2.398	15
2.361	15
2.327	15
2.034	20
1.979	15
1.935	20
1.912	50
1.796	15
1.751	10
1.711	20
1.619	10
1.596	20
1.574	15

Sodium Zirconium Fluoride
 γ $2\text{NaF} \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
4.98	100
4.37	50
4.19	80
3.96	50
3.45	50
3.36	60
3.16	40
3.07	80
2.839	70
1.843	50

Sodium Zirconium Fluoride
 $7\text{NaF} \cdot 6\text{ZrF}_4$ (5)

$d(\text{\AA})$	I/I_1
7.37	20
6.86	10
5.07	10
4.85	5
4.37	20
4.06	23
3.98	5
3.69	10
3.55	5
3.45	40
3.25	5
3.13	100
2.85	5
2.72	15
2.64	5
2.37	5
2.32	5
2.19	5
2.09	10
2.03	10
2.00	15
1.95	15
1.92	100
1.91	100
1.86	15
1.81	10
1.79	10
1.74	10
1.70	10
1.68	10
1.63	50
1.61	5
1.58	5
1.56	10
1.51	15
1.48	10

Sodium Zirconium Fluoride
 $\text{NaF} \cdot \text{ZrF}_4$ (2)

$d(\text{\AA})$	I/I_1
5.57	30
3.37	40
3.96	30
3.86	100
3.01	15
2.86	10
2.75	7
2.72	7
2.51	7
2.28	25
2.21	20
2.09	30
2.05	5
2.02	15
2.00	5
1.99	10
1.86	15
1.84	7
1.70	20
1.65	20
1.63	12
1.61	7
1.56	10

Sodium Zirconium Fluoride
 $3\text{NaF} \cdot 4\text{ZrF}_4$ (5)

$d(\text{\AA})$	I/I_1
7.56	15
7.42	45
5.47	15
4.15	100
3.78	20
3.74	20
3.42	25
3.39	35
3.36	60
2.630	15
2.074	75
1.935	12
1.766	50
1.506	25

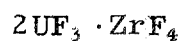
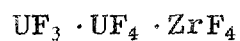
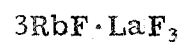
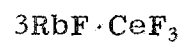
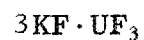
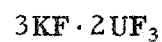
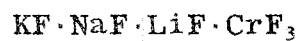
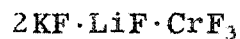
Uranium Zirconium Fluoride
 $\text{UF}_6 \cdot 3\text{ZrF}_4$

$d(\text{\AA})$	I/I_1
6.15	35
4.11	100
3.95	20
3.88	8
3.72	75
3.44	35
3.22	20
3.17	35
2.77	12
2.69	30
2.51	25
2.29	20
2.25	17
2.12	12
2.06	85
2.02	10
2.01	10
1.98	8
1.95	10
1.92	35
1.86	30
1.84	35
1.81	20
1.77	20
1.73	20
1.68	15
1.64	5
1.62	7
1.59	7
1.58	7
1.54	10

Zinc Zirconium Fluoride
 $\text{ZnF}_2 \cdot \text{ZrF}_4$

<u>d(Å)</u>	<u>I/I₁</u>
4.68	5
4.49	35
4.15	5
4.06	100
3.55	15
3.15	15
2.852	50
2.226	15
2.008	35
1.989	20
1.815	10
1.796	65
1.793	50
1.638	30

B. X-ray diffraction patterns for the compounds below are listed in this section. The purity of these compounds has never been absolutely established, nor have these compounds been isolated as single phases.



Potassium Lithium Chromium (III)
Fluoride $2\text{KF} \cdot \text{LiF} \cdot \text{CrF}_3$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
4.61	75
3.33	20
2.95	15
2.822	90
2.667	15
2.482	15
2.407	30
2.327	30
2.303	90
2.012	45
1.993	100
1.672	15
1.628	40
1.536	15

Potassium Sodium Lithium Chromium (III) Fluoride
 $\text{KF} \cdot \text{NaF} \cdot \text{LiF} \cdot \text{CrF}_3$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
4.74	45
4.09	10
2.90	100
2.478	15
2.373	55
2.321	20
2.052	85
2.010	30
1.676	40
1.582	10

Potassium Sodium Chromium (III)
Fluoride $2\text{KF} \cdot \text{NaF} \cdot \text{CrF}_3$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
4.78	30
4.14	20
2.93	95
2.495	10
2.385	65
2.292	5
2.069	100
1.688	55

Potassium Uranium Fluoride
 $3\text{KF} \cdot 2\text{UF}_3$

$\overset{\text{O}}{d(\text{\AA})}$	I/I_1
5.37	60
4.67	25
3.43	90
3.25	100
2.97	60
2.79	20
2.73	20
2.33	20
2.10	80
1.98	40
1.79	75
1.71	20
1.53	20
1.36	35

Potassium Uranium Fluoride
 $3\text{KF} \cdot \text{UF}_3$

$d(\text{\AA})$	I/I_1
6.27	70
5.68	30
5.24	100
3.69	70
3.47	40
3.24	50
2.88	20
2.60	80
2.50	20
2.164	30
2.074	15
1.955	20
1.928	30
1.840	25
1.730	20

Rubidium Lanthanum Fluoride
 $3\text{RbF} \cdot \text{LaF}_3$

$d(\text{\AA})$	I/I_1
4.93	30
3.66	30
3.47	20
3.40	20
3.30	90
3.11	60
2.821	100
2.344	40
2.237	20
2.206	15
2.184	20
1.991	40
1.905	30
1.701	40
1.627	20

Rubidium Cerium Fluoride
 $3\text{RbF} \cdot \text{CeF}_3$

$d(\text{\AA})$	I/I_1
5.91	15
4.93	15
3.68	25
3.58	20
3.45	45
3.31	100
3.24	55
3.21	35
3.05	15
2.608	15
2.522	40
2.355	45
2.296	20
2.088	10
2.060	10
1.968	10
1.943	10
1.924	25
1.905	15
1.882	25
1.840	15
1.812	15
1.789	10
1.694	15

Uranium Zirconium Fluoride
 $\text{UF}_3 \cdot \text{UF}_4 \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
6.42	15
4.07	100
3.98	65
3.58	12
3.39	40
3.22	30
3.01	40
2.63	20
2.08	50
2.02	12
1.98	15
1.94	12
1.89	50
1.80	25
1.54	20

Uranium Zirconium Fluoride
 $2\text{UF}_3 \cdot \text{ZrF}_4$

$d(\text{\AA})$	I/I_1
4.05	100
3.98	25
3.58	15
3.39	40
3.22	35
3.00	40
2.63	15
2.07	40
2.02	12
1.94	30
1.89	40
1.84	12
1.79	25

Footnotes

1. This compound is rhombohedral and is isostructural with SiO_2 .
2. This compound has only metastable existence in a system of its own composition.
3. The original measurements on this material were made by P. A. Agron (Chemistry Division), B. S. Borie, Jr., and R. M. Steele (Metallurgy Division).
4.
 - a. This compound has been reported by W. H. Zachariasen, J. Am. Chem. Soc. 70, 2147-51 (1948)
 - b. This compound was reported by W. H. Zachariasen, idem., to be $\text{KF} \cdot \text{UF}_4$.
 - c. This compound was reported by W. H. Zachariasen, idem., to be $\alpha\text{-2NaF} \cdot \text{UF}_4$.
 - d. This compound was reported by W. H. Zachariasen, idem., to be $\text{NaF} \cdot \text{UF}_4$.
5. The original ORNL measurements on this material were made by P. A. Agron (Chemistry Division), B. S. Borie, Jr., and R. M. Steele (Metallurgy Division). The compound formula was established at a later date by the authors.
6. A graphical representation of a Debye-Scherrer pattern for this compound is reported by Wagner and Balz, Z. Electrochem., 56, 576 (1952).

Compound	dA°			I/I_1			Page
$3KF \cdot 2NaF \cdot 5ZrF_4$	8.51	7.70	3.86	100	100	100	35
$RbF \cdot NaF \cdot UF_4$	8.12	3.26	2.034	100	80	75	41
$KF \cdot LaF_3$	7.77	2.747	5.61	100	100	70	33
$B \cdot 32NaF \cdot UF_4$	7.25	4.28	2.99	100	75	60	54
$RbF \cdot UF_4$	6.86	3.43	3.46	100	100	50	43
$2KF \cdot NiF_2$	6.51	2.173	1.999	100	100	55	34
$B \cdot KF \cdot ZrF_4$	6.32	3.15	1.579	100	100	70	38
$2RbF \cdot UF_4$	6.03	3.49	1.963	100	100	65	43
$KF \cdot TeF_4 \cdot H_2O$	5.64	4.27	3.575	100	100	75	36
$NaF \cdot HfF_4$	5.61	3.87	3.13	100	100	85	50
$NaF \cdot 2UF_4$	5.61	3.26	3.08	100	70	65	56
$2NaF \cdot THF_4$	5.17	2.99	2.590	100	70	55	52
$B3NaF \cdot UF_4$	5.15	2.97	1.718	100	100	85	53
$B \cdot 32NaF \cdot ZrF_4 (3)$	5.12	4.55	2.893	100	100	100	57
$B \cdot 22NaF \cdot UF_4$	5.12	1.730	2.121	100	100	90	53
$\gamma 2NaF \cdot ZrF_4$	4.98	4.19	3.07	100	100	80	58
$4LiF \cdot UF_4$	4.93	4.44	5.13	100	100	70	29
$\gamma \cdot 2NaF \cdot UF_4$	4.92	1.967	1.669	100	100	80	54
$3KF \cdot 3NaF \cdot 2ZrF_4$	4.90	2.72	3.78	100	90	75	35
$\alpha \cdot 3NaF \cdot UF_4$	4.87	3.15	3.85	100	75	50	53
$3LiF \cdot UF_4$	4.41	4.43	3.60	100	100	80	29
$NaF \cdot 2LiF \cdot CrF_3$	4.36	3.08	1.947	100	60	40	51
$2LiF \cdot ZrF_4$	4.29	3.15	2.19	100	100	60	31
$3LiF \cdot CrF_3$	4.16	2.176	4.29	100	80	45	28
$3NaF \cdot 4ZrF_4 (5)$	4.15	2.074	2.630	100	75	60	59

Compound	dA°			I/I_1			Page
$UF_3 \cdot 2ZrF_4$	4.11	2.06	3.72	100	85	75	59
$CrF_2 \cdot ZrF_4$	4.09	2.065	4.00	100	65	45	28
$ZnF_2 \cdot ZrF_4$	4.06	1.796	2.852	100	65	50	60
$FeF_2 \cdot ZrF_4$	4.04	1.805	2.016	100	65	50	28
$3KF \cdot 2ZrF_4$	3.97	3.33	1.979	100	100	100	37
$NiF_2 \cdot ZrF_4$	3.91	1.767	2.805	100	55	50	32
$\alpha-KF \cdot ZrF_4$	3.86	4.40	5.83	100	80	60	38
$NaF \cdot ZrF_4$ (2)	3.86	3.37	5.57	100	40	30	59
$NaF \cdot NiF_2$	3.85	1.924	2.723	100	100	50	52
$LiF \cdot 4UF_4$	3.78	4.25	3.52	100	90	90	30
$CsF \cdot ZrF_4$	3.73	3.62	3.26	100	85	85	27
$2CsF \cdot ZrF_4$	3.73	3.20	2.43	100	40	40	26
CrF_3	3.62	4.00	1.649	100	30	30	27
$2RbF \cdot ZrF_4$	3.590	2.338	3.080	100	40	34	45
$2CsF \cdot UF_4$	3.55	3.44	2.03	100	100	55	25
$RbF \cdot 3UF_4$	3.52	2.002	3.36	100	100	80	44
$7RbF \cdot 6UF_4$	3.51	2.140	3.05	100	50	45	43
$2RbF \cdot 3UF_4$	3.50	2.038	5.80	100	60	45	44
$3CsF \cdot LaF_3$	3.49	3.62	4.00	100	100	80	25
$RbF \cdot 6UF_4$	3.47	3.93	2.030	100	75	75	45
$RbF \cdot BeF_2$	3.46	3.38	3.12	100	100	100	40
$\alpha \cdot RbF \cdot ZrF_4$	3.45	3.42	3.34	100	100	100	46
$5RbF \cdot 4ZrF_4$	3.44	3.42	3.36	100	100	100	46
$3RbF \cdot 3NaF \cdot 4ZrF_4$	3.44	3.11	1.861	100	100	85	48
$7KF \cdot 6UF_4$	3.44	2.096	2.111	100	80	70	37
$RbF \cdot UF_3$	3.43	2.253	1.898	100	40	40	49
$RbF \cdot LaF_3$	3.43	2.25	1.87	100	40	40	41

Compound	dA°			I/I ₁			Page
B-RbF-ZrF ₄	3.42	3.36	3.325	100	100	100	47
3RbF·UF ₄	3.40	1.959	5.56	100	60	35	42
RbF·NaF·2ZrF ₄	3.35	3.71	4.13	100	60	50	48
KF·NaF·ZrF ₄	3.34	4.09	4.85	100	65	60	36
3RbF·ZrF ₄	3.290	1.900	2.326	100	100	60	45
B4 2NaF·ZrF ₄	3.25	5.12	4.00	100	80	70	58
7NaF·6UF ₄	3.25	3.33	4.32	100	85	70	55
2CsF·BeF ₂	3.23	3.08	3.62	100	80	60	24
BeF ₂	3.21	2.367	2.189	100	100	100	24
CsF·BeF ₂	3.20	5.43	3.00	100	50	40	25
5NaF·3UF ₄	3.19	1.964	1.684	100	65	65	55
3LiF·4ZrF ₄	3.16	3.90	2.194	100	95	80	32
KF·2NaF·UF ₄	3.16	3.13	4.44	100	100	90	34
3RbF·CrF ₃	3.16	3.13	3.11	100	55	55	40
NaF·6ZrF ₄ (5)	3.13	1.92	1.91	100	100	100	58
NaF·LaF ₃	3.11	2.09	2.194	100	100	90	51
B-2 2NaF·ZrF ₄ (3)	3.11	1.912	5.47	100	100	80	57
RbF·2BeF ₂	3.10	6.16	3.39	100	70	40	40
B-1 2NaF·ZrF ₄ (3)	3.09	1.890	5.15	100	100	55	57
NaF·UF ₃	3.09	1.779	2.179	100	75	55	53
3NaF·HfF ₄	3.07	4.27	1.872	100	90	75	50
2RbF·BeF ₂	3.07	2.95	2.556	100	100	90	39
3NaF·ZrF ₄ (3)	3.06	4.75	5.25	100	75	35	57
3KF·CrF ₃	3.03	2.135	4.95	100	55	35	33
KF·BeF ₂	3.01	3.23	5.99	100	90	60	33
NaF·CrF ₂	3.01	2.039	1.975	100	25	20	49
3RbF·3NaF·2ZrF ₄	3.00	4.32	3.22	100	55	55	42

<u>Compound</u>	<u>dA°</u>			<u>I/I₁</u>			<u>Page</u>
KF•2BeF ₂	3.00	3.31	3.66	100	60	15	33
7LiF•6UF ₄	2.99	5.24	3.33	95	90	90	30
CrF ₂	2.97	3.35	2.805	100	50	30	27
KF•NaF•BeF ₂	2.786	2.367	2.287	100	100	70	34
NaF•CeF ₃	2.57	3.09	1.777	100	90	90	49
3KF•BeF ₃	2.39	2.98	2.27	100	75	70	32
RbF•NaF ZrF ₄	2.152	2.094	3.39	100	100	65	49
3LiF•ZrF ₄	2.07	5.49	4.88	100	55	50	31
NaF•TeF ₂	1.964	3.92	2.78	100	90	50	51
3RbF•BeF ₂	1.425	1.421	2.95	100	100	60	39

