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**The crystal structure of  $\beta$ -KCeF<sub>4</sub>\***. By GEORGE BRUNTON, *Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, U.S.A.*

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The crystal structure of  $\beta$ -KCeF<sub>4</sub> has been determined by X-ray diffraction. The space group is *Pnma*,  $a_0 = 6.2895 \pm 0.0003$ ,  $b_0 = 3.8040 \pm 0.0003$ ,  $c_0 = 15.596 \pm 0.002$  Å. The structure consists of a three-dimensional framework of 9-coordinated Ce-F and K-F polyhedra.

Alkali metal complexes with the rare earth fluorides are being studied because of their relationship to the corresponding actinide elements which are of interest to molten salt breeder reactor technology. Cerium is analogous in its properties to plutonium and a preliminary study of the

phase relationships in the system KF-CeF<sub>3</sub> (Barton, Brunton, Hsu & Insley, 1967) showed that there are two stable phases of KCeF<sub>4</sub>:  $\alpha$ -KCeF<sub>4</sub>, fluorite-cubic and  $\beta$ -KCeF<sub>4</sub>, orthorhombic.

$\beta$ -KCeF<sub>4</sub> is the first polymorph of orthorhombic symmetry which has been described. Zachariasen (1948*a, b*) described compounds  $\beta_1$ -KLaF<sub>4</sub> and  $\beta_1$ -KCeF<sub>4</sub> and reported them to be isostructural with  $\beta_1$ -K<sub>2</sub>UF<sub>6</sub> which has *P* $\bar{6}2m$  symmetry. Sears (1967) has determined the crystal structure

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Table 1. Atomic parameters for  $\beta$ -KCeF<sub>4</sub>

	<i>x</i>	<i>y</i>	<i>z</i>	$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
Ce	0.25105 (0.4)	0.25	0.43765 (0.2)	0.00338 (0.8)	0.0077 (2)	0.00072 (0.1)	0.0	-0.00002 (0.1)	0.0
K	0.2766 (3)	0.75	0.20178 (0.9)	0.0046 (2)	0.0250 (8)	0.00104 (0.4)	0.0	0.00008 (0.7)	0.0
F(1)	0.1376 (6)	0.25	0.0364 (3)	0.0060 (7)	0.020 (30)	0.0015 (2)	0.0	0.0004 (3)	0.0
F(2)	-0.0053 (6)	0.75	0.4406 (2)	0.0062 (8)	0.018 (30)	0.0009 (2)	0.0	0.0002 (2)	0.0
F(3)	0.3970 (7)	0.75	0.3638 (3)	0.0095 (8)	0.010 (20)	0.0013 (2)	0.0	0.0008 (3)	0.0
F(4)	0.0849 (7)	0.25	0.3044 (3)	0.0131 (9)	0.015 (20)	0.0012 (2)	0.0	-0.0003 (3)	0.0

\* Coefficients in the temperature factor;  $\exp [-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$ . The number in parentheses is  $\sigma \times 10^4$ .

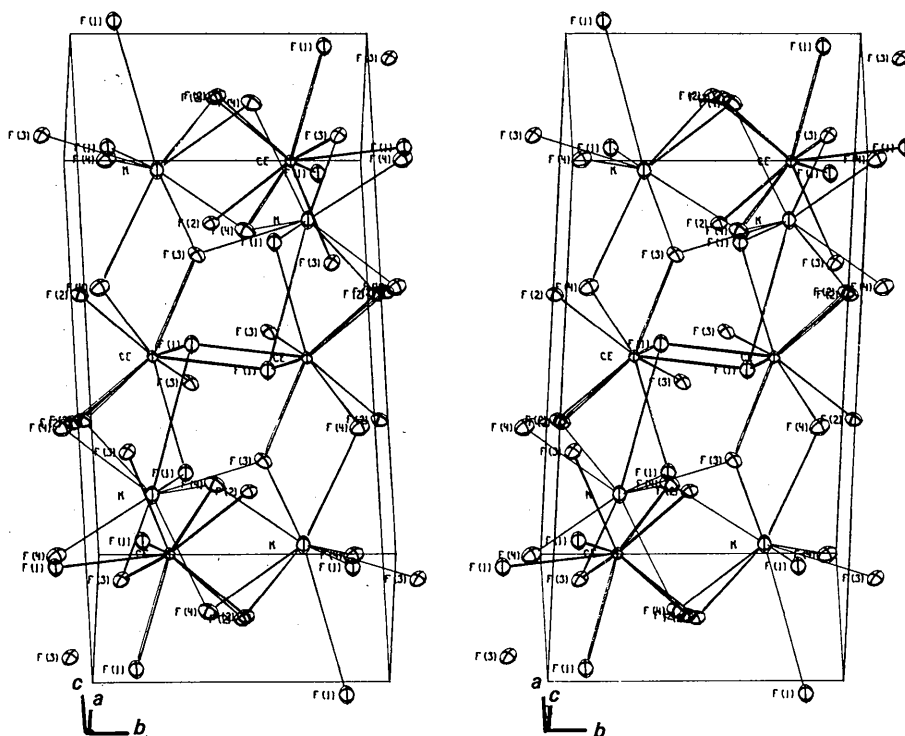


Fig. 1. The contents of one unit cell (outlined) of  $\beta$ -KCeF<sub>4</sub> tilted 45° around  $a_0$ .



