

(In the parallel setting of the double crystal X-ray spectrometer,  $Z$ =total number of electrons in the unit cell,  $\theta_0$  is the Bragg angle and  $\delta$  is the unit decrement of refractive index of the crystal.)

These X-ray diffraction intensity and peak width measurements show that the (111) plane of  $\gamma\text{-CuI}$  contains  $\text{Cu}^+$  ions while the (111) plane contains  $\text{I}^-$ . Moreover, the studies showed that the natural faces of the tetrahedral crystals were of the (111) index. This study demonstrates the feasibility of working with single crystals as small as 1 mm in diameter for direct crystallographic polarity determinations using a double crystal X-ray spectrometer.

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**Ce<sub>2</sub>O<sub>2</sub>Sb and Ce<sub>2</sub>O<sub>2</sub>Bi crystal structure.\*** By R. BENZ, *Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico 87544, U.S.A.*

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Ce<sub>2</sub>O<sub>2</sub>Sb and Ce<sub>2</sub>O<sub>2</sub>Bi crystals were prepared with body-centered tetragonal (U<sub>2</sub>N<sub>2</sub>Sb type structure, space group I4/mmm) unit-cell parameters

	$a_0$	$c_0$	$u$
Ce <sub>2</sub> O <sub>2</sub> Sb	$4.012 \pm 0.001 \text{ \AA}$	$13.697 \pm 0.008 \text{ \AA}$	$0.344 \pm 0.003$
Ce <sub>2</sub> O <sub>2</sub> Bi	$4.034 \pm 0.001$	$13.736 \pm 0.002$	$0.344 \pm 0.003$

Compounds with the chemical formula Ce<sub>2</sub>O<sub>2</sub>X, X=Sb and Bi, were prepared by reaction of weighed quantities of fused Ce<sub>2</sub>O<sub>3</sub>+Ce and of elemental X in sealed silica capsules for one month at 800°. X-ray diffraction powder patterns of the two products could be indexed on the basis of tetragonal symmetry. Unit-cell dimensions and densities calculated for two molecules per unit cell are listed in Table 1.

\* Work done under the auspices of the U.S. Atomic Energy Commission.

The powder patterns are similar to that of the U<sub>2</sub>N<sub>2</sub>Sb type previously reported for U and Th compounds (Benz & Zachariasen, 1970) and to Ce<sub>2</sub>O<sub>2</sub>Te (Pardo & Flahaut, 1962). Accordingly, the structure is

Space group I4/mmm ( $D_{4h}^{17}$ )  
 (000)  $(\frac{1}{2}\frac{1}{2}\frac{1}{2}) + 2X$  on (000)  
 4Ce in  $\pm(00u)$   
 4O in  $\pm(\frac{1}{2}0\frac{1}{4})$

where from observed intensities the parameter value was

Table 1. Lattice-parameter data and densities of Ce<sub>2</sub>O<sub>2</sub>X compounds

	$a_0$	$b_0$	$u$	$v$	Reference	Density (g.cm <sup>-3</sup> )
Ce <sub>2</sub> O <sub>2</sub> Sb	$4.012 \pm 0.001 \text{ \AA}$	$13.697 \pm 0.008 \text{ \AA}$	$0.344 \pm 0.003$	—	This work	$6.540 \pm 0.007$
Ce <sub>2</sub> O <sub>2</sub> Bi	$4.034 \pm 0.001$	$13.736 \pm 0.002$	$0.344 \pm 0.003$	—	This work	$7.747 \pm 0.02$
Ce <sub>2</sub> O <sub>2</sub> Te	$4.0705 \pm 0.0006$	$12.904 \pm 0.002$	$0.344 \pm 0.003$	—	This work	$6.835 \pm 0.004$
Ce <sub>2</sub> O <sub>2</sub> S	$4.09$	$12.92$			Pardo & Flahaut (1962)	$6.76$
	$4.001 \pm 0.002$	$6.844 \pm 0.006$	$0.278 \pm 0.003$	0.63	This work	$6.028 \pm 0.01$
	$4.01 \pm 0.01$	$6.83 \pm 0.03$	$0.29 \pm 0.02$	0.64	Zachariasen (1949)	5.99
	$4.00$	$6.87$	—	—	Flahaut & Guittard (1955)	6.00
	$4.004$	$6.872$	—	—	Picon & Patrie (1956)	6.00
	$4.008$	$6.886$	$0.208$	0.863	Flahaut, Guittard & Patrie (1958)	5.98
Ce <sub>2</sub> O <sub>2</sub> Se	$4.0152 \pm 0.0003$	$7.0492 \pm 0.0009$	$0.293 \pm 0.003$	0.63	This work	$6.603 \pm 0.002$
	$4.04 \pm 0.01$	$7.06 \pm 0.01$	—		Benacerraf, Guittard, Domange & Flahaut (1959)	6.51

determined as being  $\mu = 0.344 \pm 0.003$ . Nearest-neighbor interatomic distances are listed in Table 2.

Table 2. Nearest-neighbor interatomic distances in  $\text{Ce}_2\text{O}_2\text{X}$  compounds

	Ce-4O, ( $\pm 0.02$ Å)	Ce-3X, ( $\pm 0.02$ Å)
$\text{Ce}_2\text{O}_2\text{S}$	2.39	2.99
$\text{Ce}_2\text{O}_2\text{Se}$	2.38	3.10
	Ce-4O	Ce-4X
$\text{Ce}_2\text{O}_2\text{Te}$	2.37	3.51
$\text{Ce}_2\text{O}_2\text{Sb}$	2.38	3.55
$\text{Ce}_2\text{O}_2\text{Bi}$	2.39	3.58

Compounds with the analogous compositions  $\text{M}_2\text{N}_2\text{S}$  and  $\text{M}_2\text{N}_2\text{Se}$ , with  $\text{M}=\text{Th}$  and  $\text{U}$  (Benz & Zachariasen, 1969), and  $\text{Ce}_2\text{O}_2\text{S}$  (Zachariasen, 1949) and  $\text{Ce}_2\text{O}_2\text{Se}$  (Benacerraf, Guittard, Domange & Flahaut, 1959) have been reported with a structure distinct from the above with hexagonal symmetry. Crystal structure data on the latter Ce compounds are summarized in Tables 1 and 2. Compounds  $\text{M}_2\text{N}_2\text{P}$  and  $\text{M}_2\text{N}_2\text{As}$ , with  $\text{M}=\text{U}$  and  $\text{Th}$  also exist with this same structure (Benz & Zachariasen, 1970) and one might expect that compounds  $\text{Ce}_2\text{O}_2\text{P}$  and  $\text{Ce}_2\text{O}_2\text{As}$  might exist with this hexagonal structure too. However, all

attempts to prepare these two compounds were unsuccessful. Presumably, insufficient energy is gained when  $\text{Ce}^{3+}$  is promoted to the  $\text{Ce}^{4+}$  state with formation of  $\text{X}^{3-}$  ( $\text{X}=\text{P}$  and  $\text{As}$ ) ions as would be required to stabilize the compounds under our experimental conditions (ca. 800°).

We made attempts to replace O by N atoms in the crystal lattice of the various Ce compounds by heating selected  $\text{Ce}_2(\text{O}, \text{N})_2\text{X}$  mixtures in  $\text{N}_2$ . No significant change of unit-cell dimensions of the compounds in the product mixtures was observed.

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**Structure cristalline de  $\text{RbAlSi}_3\text{O}_8$ .** Par MADELEINE GASPERIN, Laboratoire de Minéralogie-Cristallographie associé au CNRS, Faculté des Sciences, Tour 16, 9 quai Saint-Bernard, 75-Paris 5, France

(Reçu le 24 novembre 1970)

The crystal structure of rubidium feldspar  $\text{RbAlSi}_3\text{O}_8$  has been refined by the least-square method. The final  $R$  factor is 0.07 for the isotropic refinement. Atomic coordinates, interatomic distances and angles show that the structure is very similar to that of sanidized orthoclase: Al and Si are disordered over the tetrahedral sites.

Des monocristaux de  $\text{RbAlSi}_3\text{O}_8$  de type feldspath ont été obtenus par Ghélis (1970) par cristallisation, pendant une semaine, d'un gel de cette composition à 600° et 1000 bars dans un tube en or scellé. Leurs dimensions comprises entre 50 et 80  $\mu$  rendent possible une étude par diffraction des rayons X.

Nous avons utilisé un diffractomètre automatique Nonius pour mesurer, par la méthode d'intégration  $\theta/2\theta$ , 771

réflexions indépendantes telles que  $F_{\theta}\text{min} \geq F_{\theta}\text{max}/10$  avec la radiation Mo  $K\alpha$  pour  $\theta$  compris entre 0 et 35°.

Les paramètres sont  $a=8,820$ ,  $b=12,992$ ,  $c=7,161$  Å,  $\beta=116,24^\circ$ . Le groupe spatial est  $C2/m$  avec  $Z=4$ .

Nous avons introduit les coordonnées atomiques trouvées par Colville & Ribbe (1968) pour l'orthose comme point de départ d'un affinement par moindres carrés sur ordinateur 360 IBM d'après le programme de Busing &

Tableau 1. Coordonnées atomiques, en fraction de maille, et facteurs de température isotropes

Les écarts-type (entre parenthèses) portent sur le dernier chiffre.

Atome	$x$	$y$	$z$	$\beta$	$x$	$y$	$z$
4Rb (ou K)	0,2958 (2)	0	0,1468 (3)	1,88 (3)	0,2840	0	0,1352
8T <sub>1</sub>	0,0104 (3)	0,1904 (2)	0,2227 (4)	0,76 (4)	0,0097	0,1850	0,2233
8T <sub>2</sub>	0,7227 (3)	0,1195 (2)	0,3440 (4)	0,75 (4)	0,7089	0,1178	0,3444
4O <sub>A</sub> (1)	0	0,1525 (9)	0	1,6 (2)	0	0,1472	0
4O <sub>A</sub> (2)	0,664 (1)	0	0,283 (2)	1,7 (2)	0,6343	0	0,2858
8O <sub>B</sub>	0,832 (1)	0,1596 (6)	0,226 (1)	1,5 (1)	0,8273	0,1469	0,2253
8O <sub>C</sub>	0,0464 (9)	0,3145 (6)	0,263 (1)	1,4 (1)	0,0347	0,3100	0,2579
8O <sub>D</sub>	0,1682 (9)	0,1283 (6)	0,403 (1)	1,5 (1)	0,1793	0,1269	0,4024