equation by which the program computes $\bar{S}$ for the case of atom B riding on atom A is

$$\bar{S} = S_0 + (w_B^2 - w_A^2)/2S_0 ,$$

where w_A^2 and w_B^2 are the mean-square displacements of atoms A and B perpendicular to the bond A–B. A calculated value $\bar{S}$ less than S_0 shows that $w_B^2 - w_A^2$ is negative, as it was never intended to be, and that the assumption that B rides A is completely unjustified. If the assumption is justified according to the definition given by Busing & Levy for the riding model, $w_B^2 - w_A^2$ will necessarily be positive or zero, and the calculated $\bar{S}$ will be greater than or equal to S_0.

Of course, a positive correction computed with the program does not in itself imply that use of the riding model is justified. Justification can only be based on an analysis of the physical situation which establishes that the model is a good approximation for the particular bond in question. In this connection some further remarks are necessary concerning the misuse of the riding model in the papers cited above. Most of the bonds for which meaningless 'corrections' have been calculated are bonds within the framework structures of cage-like or basket-like borane or carborane compounds. It is obvious that the riding model is inappropriate for such bonds; they clearly do not satisfy the defining condition for applicability of the riding model that 'the vector separation be independent of the position of one of the atoms, A, ...' or the condition that ... 'if atom B is much lighter than atom A and is strongly linked only to A, the lighter atom may be thought to 'ride' on the heavier one in the manner described'. The proper way to obtain meaningful corrections for such bonds is to perform a rigid-body analysis by the method of Cruickshank (1956) or by the more general method of Schomaker & Trueblood (1968) and subsequently to apply corrections for molecular libration by the procedure outlined by Busing & Levy (1964). The simple riding model is also not applicable in general to the correction of the lengths of bonds in rings or chains.

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Crystallographic study of cerium aluminate (CeAlO₃)*. By Y. S. KIM, Bell Telephone Laboratories, Inc., Allentown, Pennsylvania, U.S.A.

Cerium aluminate, CeAlO₃, has been successfully prepared in chemically homogeneous form. The rhombohedral lattice constants, $a = 5 \cdot 327$ Å and $\alpha = 60°15'$, fall on smooth curves with those for the isostructural aluminates of La, Pr, and Nd (space group $R\bar{3}m$) investigated by Geller & Bala [Acta Cryst. (1956). 9, 1019].

Cerium aluminate, a double trioxide compound, i.e., $A^{3+}B^{3+}O_3$, is known to be one of the perovskite types. However, the synthesis of the compound in chemically homogeneous form has been unsuccessful by the usual methods because of the chemical instability of cerium trioxide. The crystal structure of CeAlO₃ has been determined by other investigators (Roth, 1957; Schneider, Roth & Waring, 1961); it is rhombohedral, space group $R\bar{3}m$, and similar to that of certain other rare earth aluminates, REAlO₃, investigated by Geller & Bala (1956). In the work of the former authors a second phase CeO was found to be present when CeAlO₃ was prepared in helium atmosphere. In the present note further refined structural data are reported for homogeneous CeAlO₃ which was successfully synthesized in vacuo.

In preparing CeAlO₃ the stable cerous oxalate, $Ce(C_2O_4)_3 \cdot xH_2O$, was used as the source of Ce^{3+}, and C.P. grade alumina was used. An intimately mixed powder,

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* Part of the M.S. degree thesis at N.C. State College (1958).

proportioned to contain a 1:1 mole ratio of Ce₂O₃ and Al₂O₃, was heated to 1600°C for one hour in a vacuum furnace (10^{-6} torr). Both microscopic and X-ray diffraction analysis of the reacted material revealed that it was single phase Ce₂O₃.

Lattice constants of the CeAlO₃ were determined from high-angle lines in the Debye–Scherrer patterns obtained with Cr $K\alpha$ radiation at room temperature.

In Table 1 good agreement can be seen between the observed and the calculated values of interplanar spacings. The very weak lines ($h + k + l =$ odd) were, however, extremely difficult to detect in the powder patterns. The lattice constants of CeAlO₃ are tabulated below:

Rhombohedral primitive cell	Triply primitive hexagonal cell	Pseudocell dimension
$a = 5 \cdot 327 \pm 4$ Å	$a = 5 \cdot 348 \pm 4$ Å	$a = 3 \cdot 774 \pm 4$ Å
$\alpha = 60° \, 15' \pm 2'$	$c = 13 \cdot 021 \pm 5$ Å	$\alpha = 90° \, 13' \pm 3'$.

The edge length of the perovskite-like 'pseudocell' (which corresponds to omission of the weak $h + k + l =$ odd reflections) is half that of the quadruple primitive face-centered

rhombohedral (approximately f.c.c.) cell, the faces of which are parallel to those of the growth rhomb of the rare earth aluminates.

Table 1. *Observed and calculated interplanar spacings* (d) *of cerium aluminate*, $CeAlO_3$

Index Rh.	Hex.	d_{obs}	d_{calc}	I_{obs}
110	01.2	3·774	3·7742	s
10$\bar{1}$	11.0 ⎱	2·674	2·6743	vs
211	10.4 ⎰		2·6632	
11$\bar{1}$	02.1 ⎱	—	2·2802	vw
210	11.3 ⎰		2·2768	
200	20·2 ⎱	2·182	2·1820	s
222	00.6 ⎰	2·170	2·1700	w–m
220	02.4	1·887	1·8871	s
20$\bar{1}$	21.1 ⎱	—	1·7351	vvw
311	20.5 ⎰		1·7306	
21$\bar{1}$	12.2 ⎱	1·685	1·6851	m
321	11.6 ⎰			
2$\bar{1}\bar{1}$	30.0 ⎱	1·542	1·5419	s
310	21.4 ⎰			
332	01.8	1·536	1·5355	w
20$\bar{2}$	22.0	—	1·3372	vw
422	20.8	1·332	1·3316	m
30$\bar{1}$	31.2	—	1·2604	vw
330	03.6 ⎱	1·258	1·2581	v–m
411	30.6 ⎰			
32$\bar{1}$	13.4	1.195	1·1950	m
431	12.8	1·192	1·1920	m–s

The calculated rhombohedral cell volume and X-ray density as determined from the lattice constants are 107·9 $Å^3$ and 6·62 $g.cm^{-3}$, respectively. In Figs. 1 and 2 the lattice constants and the angles (α) for $CeAlO_3$ are compared with other rare earth aluminates as determined by Geller & Bala and by Roth. Schneider, Roth & Waring (1961) quote the Geller & Bala results for the La, Pr, and Nd aluminates but quote Roth's results for the Ce aluminate. The primitive rhombohedral cell dimensions for $CeAlO_3$ obtained in the present study are seen to be larger than those obtained by Roth but are in good agreement with the trend of other aluminates determined by Geller & Bala (1956).

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Schneider, S. J., Roth, R. S. & Waring, J. L. (1961). *J. Res. Nat. Bur. Stands.* A, 65, 345.

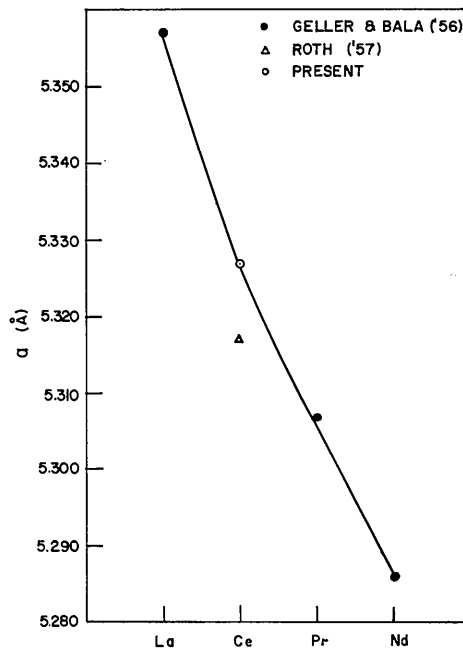Fig. 1. Plot of the lattice constant, a, of the primitive rhombohedral cell of rare earth aluminates ($REAlO_3$, Re = La, Ce, Pr, Nd). The value for $CeAlO_3$ determined by Roth was converted from the pseudocell to the primitive cell dimension.
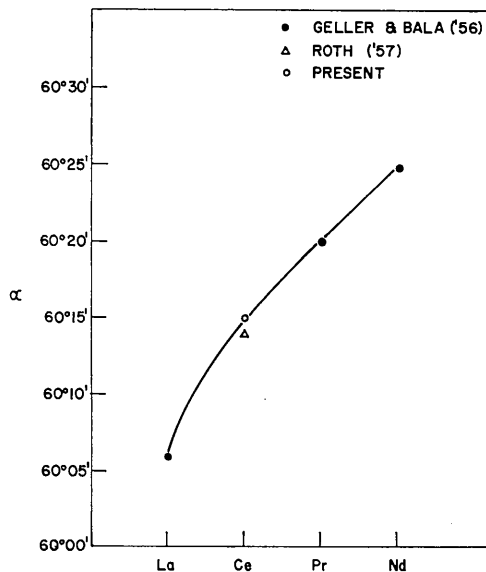

Fig. 2. Plot of the angle, α, of the primitive rhombohedral cell of rare earth aluminates ($REAlO_3$, RE = La, Ce, Pr, Nd). The value for $CeAlO_3$ determined by Roth was converted from the pseudocell to the primitive cell value.