

This conformation minimizes repulsion between the three substituents. The hydroxyl and (CH₃)₃N groups are thus equatorial, the methyl substituent is axial. The maximum deviation from the cyclopentane torsion angles is 4°. The crystal is constructed from ion pairs

in which the ions are linked by an O—H...Cl hydrogen bond [O...Cl 3.096 (6), H(10)...Cl 2.33 (2) Å].

We thank the Verband der Chemischen Industrie for financial support. The *SHELXTL* program written by GMS was employed for structure determination and plotting.

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SHORT COMMUNICATIONS

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Lattice constants of the compounds Sr₂LnAlO₅ and Sr₂LnFeO₅. By M. DROFENIK and L. GOLIČ. *Institute 'Jožef Stefan', Chemistry Department, University of Ljubljana, 61000 Ljubljana, Yugoslavia*

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Abstract

Lattice parameters of the compounds Sr₂Ln(Al,Fe)O₅ were determined and the non-linearity of the r vs $V^{1/3}$ plot is discussed.

As part of the research program on the structural and magnetic properties of the compositions in the ternary system SrO–Ln₂O₃–Fe₂O₃, crystals of compounds with the general formula Sr₂Ln(Al,Fe)O₅ were prepared and the lattice parameters were redetermined. The crystals used for the lattice determination were prepared by the HST method (Drofenik, Golič & Kolar, 1979).

The cell parameters given in Table 1 were measured at 293.2 (5) K using an Enraf–Nonius CAD-4 diffractometer.

Table 1. Comparison of cell parameters (Å), ionic radii (Å) and $V^{1/3}$ (Å) for some related compounds

	a	c	$r^{\text{VIII}}r^*$	$V^{1/3}$
Sr ₂ LaAlO ₅	6.885 (1)	11.059 (1)	1.160	8.063
Sr ₂ PrAlO ₅	6.809 (1)	11.032 (1)	1.126	7.997
Sr ₂ NdAlO ₅	6.791 (1)	11.004 (1)	1.109	7.976
Sr ₂ SmAlO ₅	6.757 (1)	10.972 (2)	1.079	7.942
Sr ₂ EuAlO ₅ *	6.742 (1)	10.970 (1)	1.066	7.930
Sr ₂ GdAlO ₅	6.735 (1)	10.937 (2)	1.053	7.916
Sr ₂ TbAlO ₅	6.717 (1)	10.932 (2)	1.040	7.901
Sr ₂ SmFeO ₅	6.822 (1)	11.267 (2)		
Sr ₂ EuAlO ₅ *	6.812 (3)	11.263 (3)		
Sr ₂ GdFeO ₅	6.805 (2)	11.263 (4)		

* Already published in Drofenik & Golič (1979).

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They were determined by least-squares refinement of 45 reflection angles in the range $10 < \theta < 25^\circ$, centered at $\pm 2\theta$ using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.70930$ Å).

In Fig. 1 the plot of ionic radius, r , vs $V^{1/3}$ is presented, where V is the cell volume of the structure. Values of $r^{\text{VIII}}r^*$ were taken from the Shannon (1976) ionic radii. Good agreement was found for all rare-earth ions except La³⁺. Since the detailed structure of Sr₂LaAlO₅ was not known, one would suppose that the coordination number of La³⁺ is not similar to that of the other rare-earth ions in this isostructural series, namely eight (Drofenik & Golič, 1979).

* The convention of Shannon (1976) is followed in this paper whereby a coordination number is denoted by a preceding Roman superscript. Thus $r^{\text{VIII}}r^*$ is the effective radius of the particular species when eightfold coordinated.

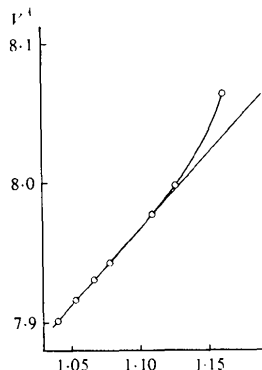


Fig. 1. r (Å) vs $V^{1/3}$ (Å) for the first seven structures in Table 1.

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The partial disorder observed in these compounds probably results because the strontium ions are larger than the rare-earth ions, and prefer the more spacious ten-coordinated 4(a) sites of space group $I4/mcm$. This does not hold for La^{3+} which may occupy ten-coordinated (8 + 2) 4(a) sites. In this case, the larger ionic radius for La^{3+} should be used, which would give better agreement in the r vs $V^{1/3}$ plot.

To obtain a more reliable basis for the discussion of this problem, the crystal structure of $\text{Sr}_2\text{LaAlO}_5$ was checked to see whether it is isostructural with the refined structure of $\text{Sr}_2\text{EuAlO}_5$ (Drofenik & Golič, 1979). We stopped the refinement at an R value of 0.11, at which point we saw exactly the same details of the structure.

This structure analysis indicates that La^{3+} occupies the 8(h) positions, coordinated by eight O atoms. The non-linearity of the r vs $V^{1/3}$ plot is thus caused by other factors. However, such plots are not always linear. For some perovskite $\text{BaM}^{4+}\text{O}_3$ compounds (where $M = \text{Ti, Tc, Sn, Hf, Zr, Pb, Pu, Np, Ce, Th}$) deviations from linearity in such plots were also found (Fukunaga & Fujita, 1973).

Similar deviations can be found for some other structures, such as $\text{Sm}_2\text{M}_2\text{O}_7$ (where $M = \text{Ti, Ru, Ir, Tc, Sn, Hf, Zr, Pb}$) (Shannon, 1974).

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Refinement of the Y_2O_3 structure at 77 K. By M. FAUCHER, *ER 210, CNRS, 92190 Meudon-Bellevue, France* and J. PANNETIER, *Institut Laue-Langevin, BP n° 156, 38042 Grenoble CEDEX, France*

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Abstract

Y_2O_3 belongs to the space group $Ia\bar{3}$ with $Z = 16$ and $a = 10.6073$ (3) Å at 77 K; the structural parameters refined from neutron powder diffraction data do not differ significantly from room-temperature values.

1. Introduction

Cubic Y_2O_3 is an attractive material for crystal-field studies. Firstly, it is an efficient phosphor host and secondly its structure is relatively simple. Nearly all the fluorescent transitions observed under ultraviolet excitation of the Eu-doped compound originate from only one of the two crystallographic sites available for the rare earth (the C_2 site). We have recently reported (Dexpert-Ghys & Faucher, 1979) the symmetry labels associated with the lower electronic levels of Eu^{3+} in the C_2 site. The optical investigations were carried out at 77 K and the final aim was the determination of crystal-field parameters, which is facilitated by the use of the results of *ab initio* calculations.

However, such calculations are extremely sensitive to tiny atomic displacements and the influence of temperature on atomic positions cannot be calculated *a priori*. The investigation by neutron powder diffraction was undertaken to determine the structural parameters of Y_2O_3 at 77 K.

The room-temperature structure of Y_2O_3 is already well known through neutron diffraction studies on single-crystal

As pointed out earlier (Shannon, 1974) it is possible that all such plots show this behavior, but it becomes more pronounced when a structure type is stable for cations which have a wide range of possible radii, and especially for compounds which contain large polarizable cations.

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(O'Connor & Valentine, 1969) or powder material (Bonnet, Delapalme & Fuess, 1975).

2. Experimental and refinement

The sample material was high purity (99.99%) Y_2O_3 (REPL) from Johnson Matthey. The powder diffraction pattern at 77 K was recorded on the D1A high-resolution spectrometer of the Institut Laue-Langevin (ILL) with $\lambda = 1.909$ Å from the (333) plane of a Ge monochromator. The powdered sample was inserted in a 15 mm diameter vanadium tube. Data were collected from $\theta = 12$ to 78° in steps of 0.05° ; the measurement time was about 30 s per step. The data from the ten counters were summed with ILL programs (Wolfers, 1970). Diffraction angles and integrated intensities were determined by fitting the shape of the Bragg peaks to Gaussian distributions and the background to a first-order polynomial. The refinement was based on 41 observed intensities (117 hkl); least-squares refinement of the cell parameter leads to $a = 10.6073$ (3) Å. The space group is $Ia\bar{3}$ with $Z = 16$ and the atoms occupy the following positions:

Y(1)	8(b)	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
Y(2)	24(d)	u	0	$\frac{1}{4}$
O	48(c)	x	y	z

The structural and thermal parameters were refined with the Busing, Martin & Levy (1962) least-squares program. The