

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 $Ia3$ 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 $Ia3$ 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

Table 1. Crystallographic parameters of Y_2O_3 at 77 and 300 K, and the scattering length of Y (e.s.d.'s in parentheses)

	u	x	y	z	$B_{Y1} (\text{Å}^2)$	$B_{Y2} (\text{Å}^2)$	$B_O (\text{Å}^2)$	R	R_w	b_{Y1} ($\times 10^{11}$ mm)	b_{Y2} ($\times 10^{11}$ mm)
Present work (77 K)	-0.0323 (2)	0.3912 (3)	0.1515 (3)	0.3800 (3)	0.25 (4)	0.37 (7)	0.36 (3)	0.038	0.038	0.770 (6)	0.770 (10)
Bonnet, Delapalme & Fuess (1975) (300 K)	-0.0326 (2)	0.3911 (2)	0.1519 (2)	0.3806 (3)	0.09*	0.305*	0.351*	0.018	-	0.764 (10)	0.765 (5)
O'Connor & Valentine (1969) (300 K)	-0.0327 (3)	0.3907 (3)	0.1520 (3)	0.3804 (3)	Anisotropic			0.105	-	0.786*	0.786*

* Not refined.

Table 2. Polar coordinates of O atoms with respect to Y in the S_6 and C_2 sites (unprimed: real case; primed: ideal fluorite case)

		Present work [$a = 10.6073$ (3) Å]					Bonnet <i>et al.</i> (1975)	
		R (Å)	θ (°)	φ (°)	R' (Å)	θ' (°)	φ' (°)	R (Å)
C_2	{	2.337 (4)	57.25	130.36 -49.64	2.2965	54.7356	135 -45	2.333
		2.268 (4)	69.03	40.63 -139.37			45 -135	2.273
		2.243 (4)	136.06	137.84 -42.15			125.2644 -45	2.239
S_6	{	2.288 (3)	62.47	-117.63 2.37 122.37	2.2965	70.5287	-120 0 120	2.289
			117.53	-177.63 -57.63 62.37			109.4713 -180 -60 60	

function minimized is $\sum_i w_i \{F_o^2(i) - \sum_{i'} m(i') [SF_c(i')]^2\}^2$, where $w_i = 1/\sigma_i^2$ is the weight of the measure, the i summation runs over the observed planes, and the i' summation over different Bragg peaks contributing to a single reflexion. $F_o^2(i)$ is the observed intensity corrected for the Lorentz factor, S is the scale factor and $F_c^2(i')$ the calculated intensity.

The variable parameters were u , x , y and z , the three isotropic thermal parameters B_{Y1} , B_{Y2} , and B_O , and the overall scale factor S . The starting u , x , y and z values were those obtained by Bonnet *et al.* (1975). Starting B_{Y1} , B_{Y2} and B_O values were set equal to zero. The scattering length for Y was that determined by Bonnet *et al.* (1975), i.e. $b_Y = 0.765 \times 10^{-11}$ mm and for O that given by Bacon (1972), $b_O = 0.580 \times 10^{-11}$ mm.

The final refined values with their e.s.d.'s are reported in Table 1. The expressions for the reliability factors are:

$$R = \frac{\sum_i |F_o^2(i) - \sum_{i'} |SF(i')|^2 m(i')|}{\sum_i F_o^2(i)},$$

$$R_w = \left(\frac{\sum_i w(i) |F_o^2(i) - \sum_{i'} |SF(i')|^2 m(i')|^2}{\sum_i w_i |F_o^2(i)|^2} \right)^{1/2}.$$

An attempt was made to refine the scattering length of Y(1) and Y(2), assigning to the thermal parameters their best

refined values. A slight but identical change occurred for both, yielding $b_Y = 0.770$ (8); the reliability factors were not significantly improved.

Absorption corrections of the thermal parameters (Hewat, 1979) are negligible since $\mu r = 0.014$.

3. Discussion

If the e.s.d.'s are taken into account, the differences between the sets of structural parameters listed in Table 1 are insignificant.

Polar coordinates of O atoms, R (Å), θ (°), φ (°), with Y as origin have been calculated and are reported in Table 2, for both 8(b) (S_6) and 24(d) (C_2) sites. In Table 2 are also reported the Y-O distances calculated from the data of Bonnet *et al.* (1975), and the polar coordinates of ligands in the ideal fluorite case (with the same vacancies), but with $u = 0$, $x = 0.375$, $y = 0.125$, $z = 0.375$. For the C_2 site, the origin is $u.0, \frac{1}{2}$. A 90° rotation around O_Y is applied to bring the C_2 axis along Oz . For the S_6 site, the origin is $0.25, 0.25, 0.25$. Two rotations are applied to bring the S_6 axis along Oz : -45° around Oz , and -54.7356° around O_Y . The real S_6 site is twisted by 17.63° with respect to the ideal one and flattened along the S_6 axis.

In the C_2 site the displacement of the two O atoms at 2.268 Å towards the vacancies causes an appreciable opening of the O–Y–O bond (increase of θ).

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The crystal structures of nine K feldspars from the Adamello Massif (Northern Italy): erratum.

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Abstract

Table 1 of the paper by Dal Negro, De Pieri, Quareni & Taylor [*Acta Cryst.* (1978). **B34**, 2699–2707] contains incorrect values for some of the direct-cell angles and volumes. A corrected version of part of Table 1 is given.

Table 1 shows the correct values of the cell parameters for the nine K feldspars.

† Deceased 23 August 1978.

Table 1. *Corrected cell parameters*

	P2B	P2A	CA1A	P17C	A1D	CA1B	P1C	RC20C	CA1E
<i>a</i>	8.589(2) Å	8.583(2) Å	8.563(2) Å	8.567(2) Å	8.564(2) Å	8.560(2) Å	8.574(2) Å	8.567(2) Å	8.561(2) Å
<i>b</i>	13.013(7)	12.988(7)	12.990(7)	12.980(7)	12.984(7)	12.984(7)	12.962(7)	12.970(7)	12.972(7)
<i>c</i>	7.197(2)	7.202(2)	7.210(2)	7.200(2)	7.201(2)	7.209(2)	7.210(2)	7.221(2)	7.223(2)
α	90°	90°	90°	90°4'	90°8'	90°17'	90°21'	90°26'	90°34'
β	116°1'	116°3'	115°56'	116°2'	116°1'	116°2'	116°2'	116°0'	115°56'
γ	90°	90°	90°	89°45'	89°32'	89°2'	88°48'	88°29'	87°55'
α^*	90°	90°	90°	90°3'	90°5'	90°9'	90°12'	90°15'	90°23'
β^*	90°	90°	90°	90°15'	90°27'	90°56'	91°10'	91°28'	92°2'
<i>V</i>	722.9 Å ³	721.3 Å ³	721.2 Å ³	719.4 Å ³	719.5 Å ³	719.8 Å ³	719.8 Å ³	720.9 Å ³	720.9 Å ³
F_{000}	550.96	550.96	550.56	548.74	550.14	550.56	550.19	548.58	550.56
Total number of reflections	2088	2088	2047	2093	2079	2095	2091	2092	2097
Reflections with $I > 2\sigma(I)$	1638	1587	1640	1738	1907	1637	1455	1773	1737
R_{final}	3.4	3.4	3.6	3.2	2.4	3.8	5.3	3.5	2.8

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