

# Refinement of the crystal structure of praseodymium orthoscandate, PrScO<sub>3</sub>

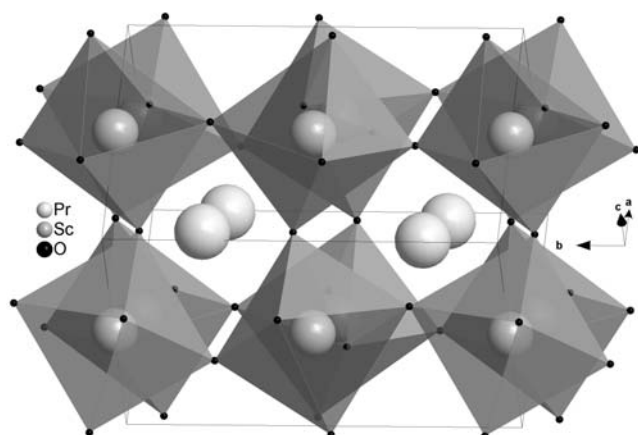
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## Abstract

O<sub>3</sub>PrSc, *Pnma* (no. 62),  $a = 5.780(1) \text{ \AA}$ ,  $b = 8.025(2) \text{ \AA}$ ,  $c = 5.608(1) \text{ \AA}$ ,  $V = 260.1 \text{ \AA}^3$ ,  $Z = 4$ ,  $R_{\text{gt}}(F) = 0.025$ ,  $wR_{\text{ref}}(F^2) = 0.060$ ,  $T = 298 \text{ K}$ .

## Source of material

A PrScO<sub>3</sub> single crystal of 30 mm in length and 15 mm in diameter was grown by the Czochralski technique with RF heating and automatic diameter control. The starting oxides Pr<sub>6</sub>O<sub>11</sub> and Sc<sub>2</sub>O<sub>3</sub> were of 99.999 % and 99.99 % purity, respectively. Due to its very high melting temperature about 2200 °C PrScO<sub>3</sub> was grown from an Ir crucible under flowing nitrogen. The pulling rate was 1 mm/h and the rotation 10 rpm. The occurrence of Pr<sup>4+</sup> ions caused a dark-brown colour of the as-grown crystal. Subsequent annealing under reducing atmosphere (5 % H<sub>2</sub> + 95 % N<sub>2</sub>) led to green colour of the crystal which is characteristic for Pr<sup>3+</sup> ions.

## Discussion

Rare-earth scandates with larger RE ions (La–Dy) have a perovskite-type crystal structure with pseudo-cubic lattice parameter between 395 and 405 pm. Those compounds which can be grown as large single crystals are suitable substrates for the growth of high-quality films of a variety of ferroelectric, multiferroic, and superconducting perovskites. Uniform strain can be achieved in sufficiently thin commensurate epitaxial films on these rare-earth scandates which allows their ferroelectric properties to be tuned. For example unstrained SrTiO<sub>3</sub> which is not ferroelectric at any temperature, has been made ferroelectric at room temperature *via* biaxial strain imposed by commensurate growth on rare-earth scandate substrates [1].

Liverovich and Mitchell have published the crystal structure of PrScO<sub>3</sub> obtained by solid state reaction which were refined from powder X-ray data using the Rietveld method [2]. Using the Czochralski technique we have grown large single crystals which were used for a single crystal structure refinement. This refinement was carried out in the standard setting space group *Pnma* instead of the non standard configuration *Pbam* as used by Liverovich and Mitchell. The positional parameters reported for *Pbam* can be transferred to *Pnma* using the symmetry operation  $\frac{1}{2}+y, z, \frac{1}{2}-x$ . Doing so, the positional parameters reported here are comparable to the former one but more precized. Additionally, we have refined all atomic positions with anisotropic displacement parameters showing a slight ellipsoidal movement of the oxygen atoms perpendicular to the metal–oxygen bonds. All metal atoms are found with a nearly isotropic displacement. The scandium atoms are octahedral coordinated by oxygen atoms with an offset of 17.50(1)° along [010] and 16.87(8)° parallel to the [1 0 1] direction of the oxygen atoms away from a linear Sc—O—Sc bond as observed in the *Pm* $\bar{3}$ *m* aristotype ABO<sub>3</sub> perovskites. The praseodymium atoms are 8-fold coordinated by oxygen atoms with distances between 234.1(5) pm and 285.2(3) pm.

**Table 1.** Data collection and handling.

Crystal:	green triangle, size 0.11 × 0.15 × 0.18 mm
Wavelength:	Mo <i>K</i> <sub>α</sub> radiation (0.71073 Å)
$\mu$ :	208.47 cm <sup>-1</sup>
Diffractometer, scan mode:	STOE IPDS I, dynamic profile intergration
$2\theta_{\text{max}}$ :	60.64°
$N(hkl)_{\text{measured}}$ , $N(hkl)_{\text{unique}}$ :	5144, 409
Criterion for $I_{\text{obs}}$ , $N(hkl)_{\text{gt}}$ :	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$ , 395
$N(\text{param})_{\text{refined}}$ :	29
Programs:	SHELXL-93 [3], DIAMOND [4]

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**Table 2.** Atomic coordinates and displacement parameters (in Å<sup>2</sup>).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>12</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>23</sub>
Pr(1)	4 <i>c</i>	0.44930(6)	¼	0.48788(6)	0.0092(3)	0.0097(3)	0.0091(3)	0	0.00065(9)	0
Sc(1)	4 <i>b</i>	0	0	½	0.0077(5)	0.0075(6)	0.0074(6)	0.0001(5)	0.0003(3)	0.0004(3)
O(1)	4 <i>c</i>	0.0395(7)	¼	0.6052(8)	0.012(2)	0.009(2)	0.011(2)	0	0.001(1)	0
O(2)	8 <i>d</i>	0.1992(5)	0.0555(4)	0.1977(5)	0.010(1)	0.014(2)	0.010(1)	0.002(1)	0.003(1)	0.001(1)

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## References

1. Uecker, R.; Velickov, B.; Klimm, D.; Bertram, R.; Bernhagen, M.; Rabe, M.; Albrecht, M.; Fornari, R.; Schlom, D. G.: Properties of rare-earth scandate single crystals (Re = Nd-Dy). *J. Cryst. Growth* **310** (2008) 2649-2658.
2. Liverovich, R. P.; Mitchell, R. H.: A structural study of ternary lanthanide orthoscandate perovskites. *J. Solid State Chem.* **177** (2004) 2188-2197.
3. Sheldrick, G. M.: SHELXL-93. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1993.
4. Brandenburg, K.: DIAMOND. Visual Crystal Structure Information System. Version 3.2. Crystal Impact, Bonn, Germany 1998.