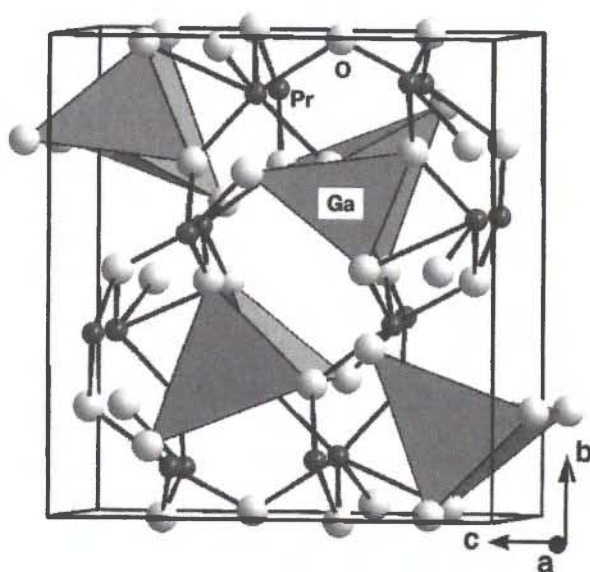


Crystal structure of praseodym gallate, $\text{Pr}_4\text{Ga}_2\text{O}_9$

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Abstract

$\text{Ga}_2\text{O}_9\text{Pr}_4$, monoclinic, $P12_1/c1$ (No. 14), $a = 7.8256(4)$ Å, $b = 11.0322(5)$ Å, $c = 11.4959(7)$ Å, $\beta = 109.187(3)^\circ$, $V = 937.4$ Å³, $Z = 4$, $R(P) = 0.026$, $wR(P) = 0.034$, $R(I) = 0.033$, $T = 295$ K.

Source of material

$\text{Pr}_4\text{Ga}_2\text{O}_9$ was synthesized by solid state reaction of the oxides of 4N and 5N quality containing Pr_2O_3 and Ga_2O_3 in a molar ratio of 2:1. The sample was sintered in air in a closed Pt crucible up to 1753 K for 20 h. This reaction led to a homogeneous product which was of light green color after grinding. Because of the incongruent melting of SrPrGaO_4 - one of the most favoured candidates for substrates for high- T_c superconductors - a shift in the melt composition during the growth process takes place. In consequence, $\text{Pr}_4\text{Ga}_2\text{O}_9$ is formed in the multiphase residual melt [1]. Starting atomic coordinates for the refinement were taken from $\text{Eu}_4\text{Al}_2\text{O}_9$ [2]. The displacement parameters of all atoms were fixed to reliable values.

Table 1. Data collection and handling.

Powder:	light-green
Wavelength:	Cu K_α radiation (1.54059 Å)
μ :	1629.9 cm ⁻¹
Diffractometer:	Stoe Stadi P
Scan mode:	transmission Debye-Scherrer mode
$2\theta_{\text{max}}$, stepwidth:	89.98°, 0.02
$N(\text{points})_{\text{measured}}$	4000
$N(\text{hkl})_{\text{measured}}$	765
$N(\text{param})_{\text{refined}}$	79
Program:	RIETAN-97 [3]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
Pr(1)	4e	0.520(2)	0.100(2)	0.782(1)	0.006
Pr(2)	4e	0.027(2)	0.091(2)	0.806(1)	0.006
Pr(3)	4e	0.332(3)	0.122(2)	0.424(2)	0.006
Pr(4)	4e	0.834(3)	0.121(2)	0.419(2)	0.006
Ga(1)	4e	0.215(5)	0.190(3)	0.137(3)	0.009
Ga(2)	4e	0.660(4)	0.184(3)	0.117(3)	0.009
O(1)	4e	0.761(9)	0.146(5)	0.804(5)	0.012
O(2)	4e	0.202(7)	0.236(4)	0.797(4)	0.012
O(3)	4e	0.176(9)	0.018(7)	0.190(7)	0.012
O(4)	4e	0.030(9)	0.219(7)	0.940(7)	0.012
O(5)	4e	0.404(8)	0.226(4)	0.083(5)	0.012
O(6)	4e	0.64(1)	0.224(8)	0.950(8)	0.012
O(7)	4e	0.737(7)	0.009(5)	0.173(4)	0.012
O(8)	4e	0.03(1)	0.020(5)	0.374(5)	0.012
O(9)	4e	0.613(9)	0.991(6)	0.390(6)	0.012

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