

Crystal structure of distrontium praseodym gallium pentaoxide, $\text{Sr}_2\text{PrGaO}_5$

Th. M. Gesing^{*I}, R. Uecker^{II} and J.-C. Buhl^I

^I Universität Hannover, Institut für Mineralogie, Welfengarten 1, D-30167 Hannover, Germany

^{II} Institut für Kristallzüchtung, Rudower Chaussee 6, D-12489 Berlin, Germany

Received February 24, 1999, transferred to 2nd update of database ICSD in 1999, CSD-No. 409415

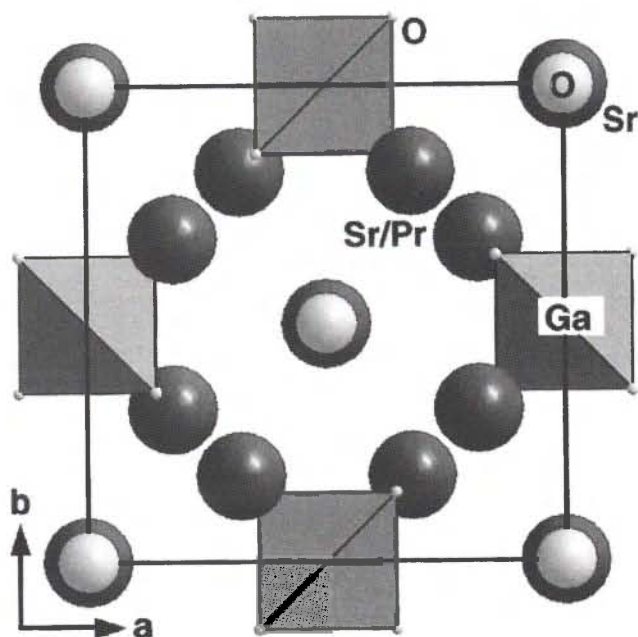


Table 1. Data collection and handling.

Powder:	brown
Wavelength:	Cu K_{α} radiation (1.54059 Å)
μ :	1008.6 cm^{-1}
Diffractometer:	Stoe Stadi P
Scan mode:	transmission Debye-Scherrer mode
$2\theta_{\text{max}}$, stepwidth:	89.98°, 0.02
$N(\text{points})_{\text{measured}}$	3500
$N(hkl)_{\text{measured}}$	67
$N(\text{param})_{\text{refined}}$	30
Program:	RIETAN-97 [3]

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

Atom	Site	Occ.	x	y	z	U_{iso}
Sr(1)	8h	0.5	0.180(2)	$x+1/2$	0	0.006
Pr(1)	8h	0.5	0.180	$x+1/2$	0	0.006
Sr(2)	4a		0	0	1/4	0.006
Ga(1)	4b		0	1/2	1/4	0.009
O(1)	4c		0	0	0	0.012
O(2)	16f		0.143(8)	$x+1/2$	0.642(5)	0.012

Abstract

$\text{GaO}_5\text{PrSr}_2$, tetragonal, $I4/mcm$ (No. 140), $a = 6.8441(2)$ Å, $c = 11.2534(4)$ Å, $V = 527.1$ Å³, $Z = 4$, $R(P) = 0.035$, $wR(P) = 0.052$, $R(I) = 0.038$, $T = 295$ K.

Source of material

$\text{Sr}_2\text{PrGaO}_5$ was synthesized by solid state reaction of the oxides and carbonates (4N and 5N quality). A mixture containing SrO , Pr_2O_3 and Ga_2O_3 in a molar ratio of 4:1:1 was used. The sample was sintered in air in a closed Pt crucible up to 1573 K for 56 h. This reaction led to a homogeneous brown product [1]. Because of the incongruent melting of SrPrGaO_4 - one of the most favoured candidates for substrates for high- T_c superconductors - primary crystallization of $\text{Sr}_2\text{PrGaO}_5$ takes place when starting the crystal growth from the stoichiometric melt composition SrPrGaO_4 .

Starting atomic coordinates for the refinement were taken from $\text{Sr}_2\text{GdGaO}_5$ [2]. The displacement parameters of all atoms were fixed to reliable values.

References

1. Uecker, R.; Reiche, P.; Ganschow, S.; Wilde, P.-M.; Uecker, D.-C.; Worzala, H.; Schultze, D.: Growth conditions and composition of SrPrGaO_4 single crystals. *J. Cryst. Growth* **174** (1997) 320.
2. Nguyen Trut Dinh; Fava, J.; le Flam, G.: Etude structurale et optique de la phase $\text{Sr}_2\text{GdGaO}_5$ dopée a l'euprium trivalent. *Z. Anorg. Allg. Chem.* **433** (1977) 275-283.
3. Izumi, F.: "The Rietveld Method", ed. by R. A. Young, Oxford University Press, Oxford (1993).

* Correspondence author

(e-mail: tm.gesing@mineralogie.uni-hannover.de)