Crystal structure of tripraseodymium hexasiliconundecanitride, $Pr_3Si_6N_{11}$

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Received May 16, 1995, transferred to database ICSD March 1996, CSD-No. 402178

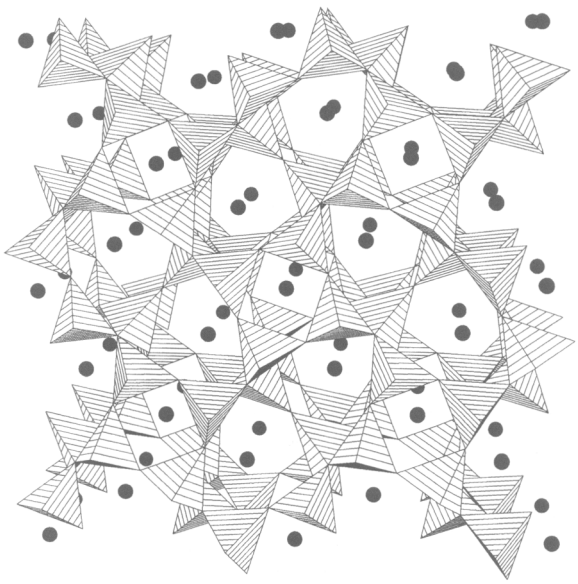

Table 1. Parameters used for the X-ray data collection

Crystal:	greenish prisma, size 0.2 x 0.15 x 0.1 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	152.94 cm^{-1}
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{measurement}$:	296 K
$2\theta_{max}$:	60°
$N(hkl)_{unique}$:	774
Criterion for F_o:	$F_o > 0\ \sigma(F_o)$
$N(param)_{refined}$:	54
Program:	SHELXTL-plus

Source of material: $Pr_3Si_6N_{11}$ was synthesized by reaction of elemental praseodymium with silicon diimide under nitrogen atmosphere at 1848 K in a high frequency furnace.
The pure compound was obtained as transparent greenish crystals. The single crystal structure determination of an isotypic compound ($Ce_3Si_6N_{11}$) is described earlier (see ref. 1). $Pr_3Si_6N_{11}$ contains Pr^{3+} as well as a polar three-dimensional covalent network of corner sharing SiN_4 tetrahedra.

$N_{11}Pr_3Si_6$, tetragonal, *P4bm* (No. 100), a =10.099(1) Å, c =4.843(1) Å, V =493.9 $Å^3$, Z =2, $R(F)$ =0.026, $R_w(F)$ =0.026.

Table 2. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pr(1)	4*c*	0.81877(3)	0.31877(3)	0.3692	0.0051(2)	U_{11}	0.0110(2)	0.0004(1)	0.0463(2)	0.0001(2)
Pr(2)	2*a*	0	0	−0.6459(2)	0.0048(2)	U_{11}	0.0079(2)	0	0	0
Si(1)	8*d*	0.0782(1)	0.2095(2)	−0.1053(4)	0.0045(7)	0.0046(6)	0.0065(7)	0.0000(4)	−0.0002(6)	0.0001(5)
N(1)	8*d*	0.0749(5)	0.2300(5)	−0.461(1)	0.006(2)	0.005(2)	0.010(2)	0.000(2)	−0.001(2)	0.001(2)
Si(2)	4*c*	0.6172(2)	0.1172(2)	−0.5947(4)	0.0038(5)	0.0038(5)	0.007(1)	−0.0006(6)	−0.0007(5)	U_{13}
N(2)	4*c*	0.6530(6)	0.1530(6)	−0.942(1)	0.008(2)	0.008(2)	0.008(2)	−0.000(2)	0.000(2)	U_{13}
N(3)	8*d*	−0.0799(5)	0.1786(5)	0.007(1)	0.006(2)	0.008(2)	0.009(2)	−0.002(2)	0.000(2)	−0.000(2)
N(4)	2*b*	1/2	0	−0.563(2)	0.010(3)	U_{11}	0.011(3)	0.002(4)	0	0

Reference

1. Schlieper, T.; Schnick, W.: Synthese, Kristallstruktur und magnetische Eigenschaften von $Ce_3Si_6N_{11}$. Z. anorg. allg. Chem. **621** (1995) 1535.