

Crystal structure of tripraseodymium hexasiliconundecanitrile, Pr₃Si₆N₁₁

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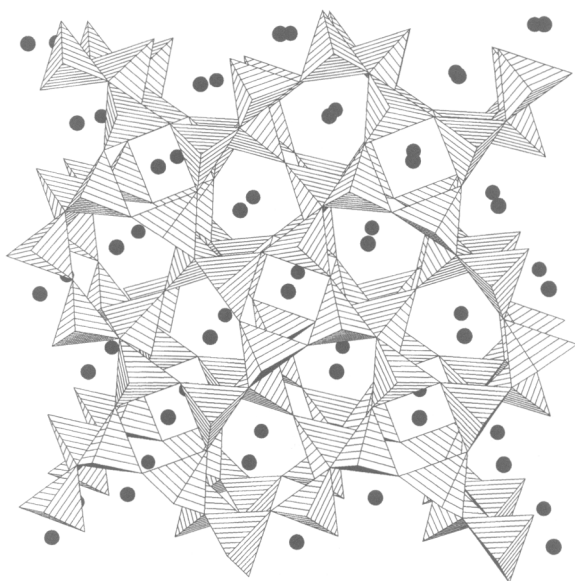


Table 1. Parameters used for the X-ray data collection

Crystal:	greenish prisma, size 0.2 x 0.15 x 0.1 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	152.94 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
T _{measurement} :	296 K
2 θ _{max} :	60°
N(hkl) _{unique} :	774
Criterion for F _o :	F _o > 0 σ (F _o)
N(param) _{refined} :	54
Program:	SHELXTL-plus

Source of material: Pr₃Si₆N₁₁ 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 isotopic compound (Ce₃Si₆N₁₁) is described earlier (see ref. 1). Pr₃Si₆N₁₁ contains Pr³⁺ as well as a polar three-dimensional covalent network of corner sharing SiN₄ tetrahedra.

N₁₁Pr₃Si₆, tetragonal, *P4bm* (No. 100), $a = 10.099(1)$ Å, $c = 4.843(1)$ Å, $V = 493.9$ Å³, $Z = 2$, $R(F) = 0.026$, $R_w(F) = 0.026$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Pr(1)	4c	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)	2a	0	0	-0.6459(2)	0.0048(2)	U ₁₁	0.0079(2)	0	0	0
Si(1)	8d	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)	8d	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)	4c	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)	4c	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)	8d	-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)	2b	1/2	0	-0.563(2)	0.010(3)	U ₁₁	0.011(3)	0.002(4)	0	0

Reference

- Schlieper, T.; Schnick, W.: Synthese, Kristallstruktur und magnetische Eigenschaften von Ce₃Si₆N₁₁. *Z. anorg. allg. Chem.* **621** (1995) 1535.