Si_3N_4	*hP*14	(176) $P6_3/m$ – h^2c

Si_3N_4 β [2]; $BeGa_2O_4$ [4]
Structural features: SiN_4 tetrahedra share vertices to form a 3D-framework with channels of hexagonal cross-section parallel to [001]. See Fig. IV.50.

Billy M. et al. (1983) [1]
N_4Si_3
a = 0.76018, c = 0.29066 nm, c/a = 0.382, V = 0.1455 nm^3, Z = 2

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Si1	6*h*	*m*..	0.2323	0.4096	$^1/_4$		tetrahedron N_4
N2	6*h*	*m*..	0.3337	0.0323	$^1/_4$		non-coplanar triangle Si_3
N3	2*c*	-6..	$^1/_3$	$^2/_3$	$^1/_4$		coplanar triangle Si_3

Experimental: powder, diffractometer, neutrons, time-of-flight, R_p = 0.052

Remarks: The only thermodynamically stable modification of Si_3N_4. Space group (173) $P6_3$ was tested and rejected in [1], however, refinements in both space groups in [3] indicated space group (173) $P6_3$ at a 95% significance level. A refinement on powder X-ray diffraction data collected on a two-phase sample (91.7 wt.% α-Si_3N_4) is reported in [3].

References: [1] Billy M., Labbe J., Selvaraj A., Roult G. (1983), Mater. Res. Bull. 18, 921-934. [2] Hardie D., Jack K.H. (1957), Nature (London) 180, 332-333. [3] Schneider J., Frey F., Johnson N., Laschke K. (1994), Z. Kristallogr. 209, 328-333. [4] Schweizer M., Müller Buschbaum H. (1979), Z. Naturforsch. B 34, 1067-1069.

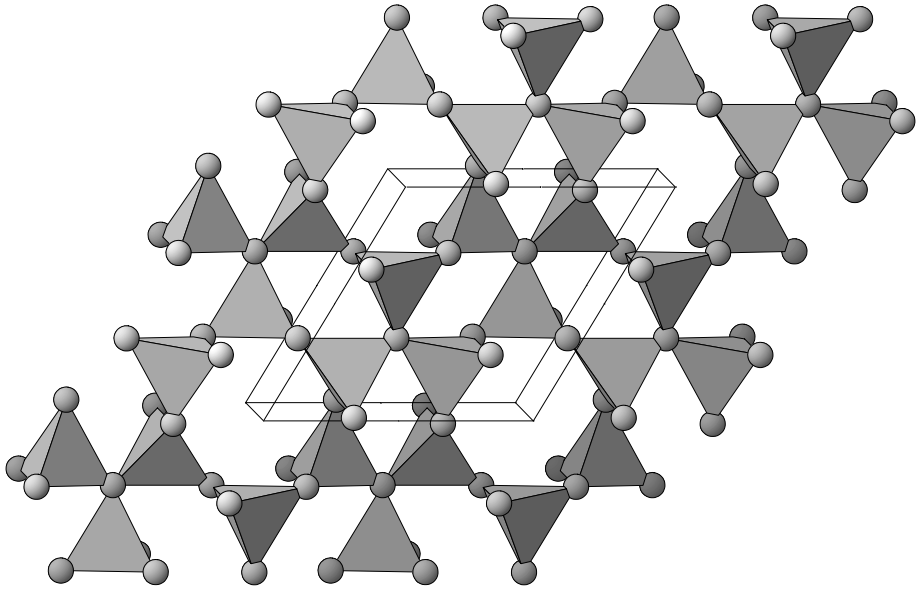

Fig. IV.50. **Si_3N_4 β**

Arrangement of SiN_4 tetrahedra.