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Crystal structure of sodium alumosilicate cyanide, $Na_8[AlSiO_4]_6(CN)_2$

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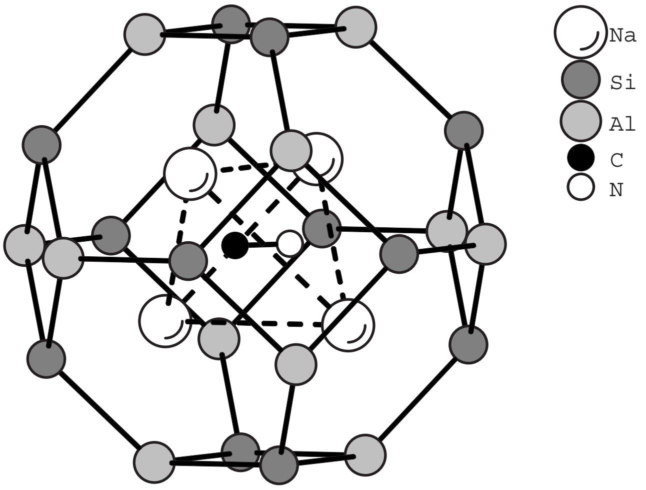

Abstract

$Al_6C_2N_2Na_8O_{24}Si_6$, cubic, $P\bar{4}3n$ (No. 218), $a = 8.9192(1)$ Å, $V = 709.5$ Å^3, $Z = 1$, $R(P) = 0.036$, $R(I) = 0.020$, $T = 293$ K.

Source of material

Samples were prepared by hydrothermal synthesis at 398 K and 24 h reaction time in 50 ml Teflon coated steel autoclaves. The alkaline transformation of kaolinite in the presence of NaCN was performed as described by Gurris [1]. The educts were mixed until a uniform slurry was formed which was then heated in the autoclaves. After the reaction period the product was washed with water and dried at 353 K for 24 h for further characterisation.

Discussion

In the past many sodalites with the general formula $Na_{6+x}[T'T''O_4]Y_x(H_2O)_{8-4x}$ for a single negative charged sodium containing framework were reported in literature. In this context we have still reported about rhodanide and cyanate containing compounds [2,3]. Here we report about our efforts to incorporate cyanide ($Y = CN^-$) anions into the β-cage of an alumosilicate sodalite ($T' = Al$, $T'' = Si$).

The crystal structure was determined from X-ray powder diffraction data. The framework of this compound corresponds to those known for other alumosilicate sodalites. The average Al—O and Si—O distances were calculated to 175 pm and 162 pm, respectively. The CN^- group was found in a linear arrangement around the centre of the cages with C—N distances of 120 pm with distinguishable positions for the carbon and nitrogen atoms. Additionally, water molecules were not found in the cages which lead to a phase composition of $Na_8[AlSiO_4]_6(CN)_2$. The IR spectrum of cyanide sodalite shows the typical symmetric and asymmetric vibration modes for the alumosilicate sodalite framework in the mid infrared region. Additionally, a single band at 2070 cm^{-1} results from the enclathration of the CN^- anions within the sodalite cages. Weak bands at 1650 cm^{-1} and between 3000 cm^{-1} – 3700 cm^{-1} are caused by adsorbed surface water, whereas a signal at 1450 cm^{-1} belongs to traces of sodium carbonate. This was formed on the outer surface of the crystals according to the reaction of residues of the mother liquor with carbon dioxide under open system conditions.

Table 1. Data collection and handling.

Powder:	white
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.071 cm^{-1}
Diffractometer, scan mode:	Stoe Stadi P, transmission, Debye-Scherrer
$2\theta_{max}$, stepwidth:	60°, 0.02°
$N(points)_{measured}$:	2750
$N(hkl)_{measured}$:	211
$N(param)_{refined}$:	31
Programs:	Rietan-97 [4], DIAMOND [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	B_{iso}
Na(1)	8*e*	1.01(1)	0.1832(6)	x	x	1.6(2)
Si(1)	6*d*		1/4	0	1/2	0.8(3)
Al(1)	6*c*		1/4	1/2	0	0.6(3)
O(1)	24*i*		0.1396(3)	0.4404(2)	0.15043(3)	0.7(2)
C(1)	12*f*	0.167	0.048(2)	0	0	1.6
N(1)	12*f*	0.167	0.913(1)	0	0	1.6

References

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