Redetermination of the crystal structure of hexaaluminium hexasilicon octasodium dichloride tetracosaoxide (sodalite), $Na_8(Al_6Si_6O_{24})Cl_2$

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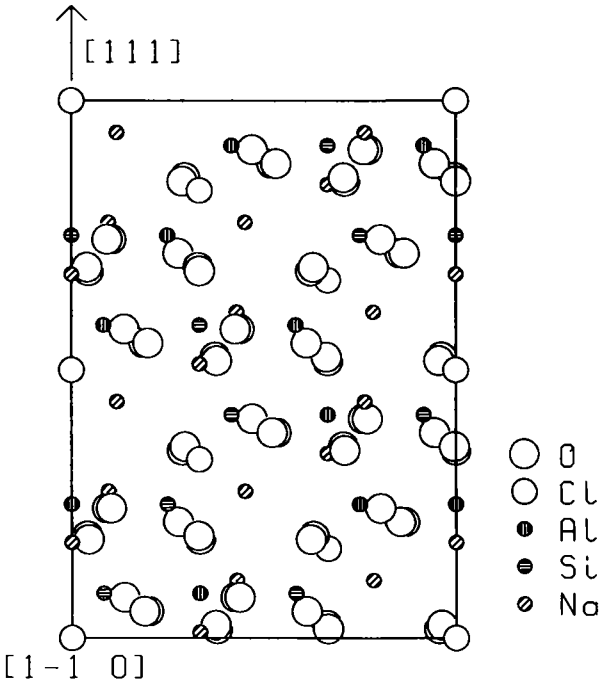

Source of material: The title compound is a natural product.
A data set of good quality was obtained on a Stoe imaging plate diffractometer (see ref. 1) for a sodalite crystal. Merging 4863 measured reflections yielded $R_{int} = 0.0202$. The strongest reflection 211 (and equivalents) was omitted, because it overloaded the imaging plate. The data set allowed the refinement of the Flack x parameter, x = –0.06(19). The coordinates agree well with ref. 2. The polarity of the [111]-direction is shown in the figure. Ignoring the bonds there are 6 layers perpendicular to the [111]-vector. Each layer has a cation-rich face towards [111] and an anion-rich face towards [$\bar{1}\bar{1}\bar{1}$].

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

Crystal:	pale blue crystal of irregular shape, size 0.27 x 0.30 x 0.38 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	9.00 cm^{-1}
Diffractometer:	Stoe IPDS
Scan mode:	100 exposures, $\Delta\varphi = 1.5°$
$T_{measurement}$:	298 K
$2\theta_{max}$:	56.1°
$N(hkl)_{unique}$:	287
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	18
Programs:	SHELXL-93, SCHAKAL

$Al_6Cl_2Na_8O_{24}Si_6$, cubic, $P\bar{4}3n$ (No. 218), a =8.873(7) Å, V =698.6 Å^3, Z =1, $R(F)$ =0.018, $R_w(F^2)$ =0.045.

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References

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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}
Al(1)	6*d*	1/4	0	1/2	0.0053(3)	0.0053(2)	U_{22}	0	0	0
Si(1)	6*c*	1/4	1/2	0	0.0045(3)	0.0056(2)	U_{22}	0	0	0
Na(1)	8*e*	0.17770(7)	*x*	*x*	0.0175(3)	U_{11}	U_{11}	0.0010(2)	U_{12}	U_{12}
Cl(1)	2*a*	0	0	0	0.0239(3)	U_{11}	U_{11}	0	0	0
O(1)	24*i*	0.13935(9)	0.14949(9)	0.4385(1)	0.0090(4)	0.0102(4)	0.0109(4)	0.0039(3)	0.0013(3)	0.0005(3)