Redetermination of the crystal structure of hexaaluminium hexasilicon octasodium dichloride tetracosaoxide (sodalite), $\text{Na}_8(\text{Al}_6\text{Si}_6\text{O}_{24})\text{Cl}_2$

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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, $\Delta\phi = 1.5^\circ$
$T_{\text{measurement}}$:	298 K
$2\theta_{\text{max}}$:	56.1°
$N(hkl)_{\text{unique}}$:	287
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	18
Programs:	SHELXL-93, SCHAKAL

$\text{Al}_6\text{Cl}_2\text{Na}_8\text{O}_{24}\text{Si}_6$, cubic, $P\bar{4}3n$ (No. 218), $a = 8.873(7)$ Å, $V = 698.6$ Å³, $Z = 1$, $R(F) = 0.018$, $R_w(F^2) = 0.045$.

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References

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- Hassan, I.; Grundy, H. D.: The crystal structures of sodalite-group minerals. *Acta Crystallogr. B* **40** (1984) 6-13.
- Sheldrick, G. M.: SHELXL-93, a program for refining crystal structures. University of Göttingen, Germany 1993.
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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 $R_{\text{int}} = 0.0202$. 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 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}
Al(1)	6d	1/4	0	1/2	0.0053(3)	0.0053(2)	U_{22}	0	0	0
Si(1)	6c	1/4	1/2	0	0.0045(3)	0.0056(2)	U_{22}	0	0	0
Na(1)	8e	0.17770(7)	x	x	0.0175(3)	U_{11}	U_{11}	0.0010(2)	U_{12}	U_{12}
Cl(1)	2a	0	0	0	0.0239(3)	U_{11}	U_{11}	0	0	0
O(1)	24i	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)