

The dehydrated copper silicate $\text{Na}_2[\text{Cu}_2\text{Si}_4\text{O}_{11}]$: a three-dimensional microporous framework with a linear Si—O—Si linkage

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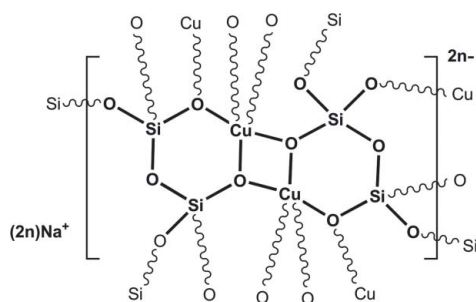
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{Si—O}) = 0.004$ Å;
R factor = 0.043; wR factor = 0.120; data-to-parameter ratio = 11.9.

The structure of the title dehydrated copper silicate, disodium dicopper undecaoxide tetrasilicate, $\text{Na}_2(\text{Cu}_2\text{O}_{11}\text{Si}_4)$, was determined by single-crystal X-ray diffraction from a non-merohedral twin. It exhibits an effective three-dimensional microporous framework with the major channels, in which the Na^+ cations are placed, running along the a -axis direction and smaller channels observed along the b -axis direction. The structure is unusual in that it contains a symmetry-constrained Si—O—Si angle of 180° . The Cu centre is coordinated to five O atoms, exhibiting a slightly distorted square-pyramidal coordination geometry. The Na cation is interacting with five neighbouring O atoms, exhibiting an uncharacteristic coordination environment.

Related literature

For related literature, see: Brandão *et al.* (2005); Haile & Wuensch (2000); Liebau (1985); Rocha & Anderson (2000); Rocha & Lin (2005); dos Santos *et al.* (2005); Ananias *et al.* (2001, 2006); Anderson *et al.* (1994); Ferreira *et al.* (2003).



Experimental

Crystal data

$\text{Na}_2(\text{Cu}_2\text{O}_{11}\text{Si}_4)$	$\gamma = 100.461$ (7)°
$M_r = 461.44$	$V = 258.9$ (2) Å ³
Triclinic, $P\bar{1}$	$Z = 1$
$a = 5.190$ (2) Å	Mo $K\alpha$ radiation
$b = 6.299$ (3) Å	$\mu = 4.71$ mm ⁻¹
$c = 8.196$ (4) Å	$T = 298$ (2) K
$\alpha = 96.390$ (7)°	$0.28 \times 0.08 \times 0.04$ mm
$\beta = 97.281$ (7)°	

Data collection

Bruker SMART CCD 1000 diffractometer	1587 measured reflections
Absorption correction: multi-scan (TWINABS; Sheldrick, 2002)	1043 independent reflections
$T_{\min} = 0.627$, $T_{\max} = 0.834$	782 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.042$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	88 parameters
$wR(F^2) = 0.119$	$\Delta\rho_{\text{max}} = 1.40$ e Å ⁻³
$S = 1.01$	$\Delta\rho_{\text{min}} = -1.58$ e Å ⁻³
1043 reflections	

Table 1

Selected bond lengths (Å).

Cu1—O5 ⁱ	1.909 (3)	Cu1—O6	1.974 (3)
Cu1—O2	1.950 (4)	Cu1—O2 ⁱⁱⁱ	2.316 (4)
Cu1—O6 ⁱⁱ	1.970 (4)		

Symmetry codes: (i) $x, y - 1, z$; (ii) $-x + 1, -y, -z + 2$; (iii) $-x + 2, -y, -z + 2$.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT-Plus (Bruker, 2003); program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXTL (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2007); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2065).

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