

Crystal structure of calcium copper phyllo-decaoxotetrasilicate, $\text{CaCuSi}_4\text{O}_{10}$

W. Bensch and M. Schur

Institut für Anorganische Chemie, Universität Frankfurt, D-60439 Frankfurt/M., Germany

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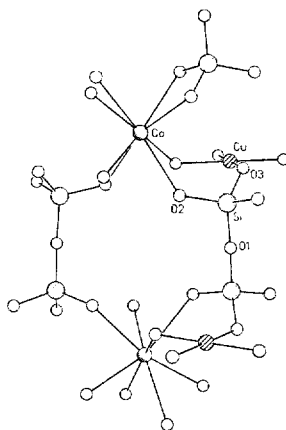


Table 1. Parameters used for the X-ray data collection

Crystal:	deep blue rectangular plate, size 0.25 x 0.25 x 0.08 mm
Wavelength:	Mo K α radiation (0.7107 Å)
μ :	39.61 cm $^{-1}$
Diffractometer:	Siemens-Stoe
Scan mode:	$\omega/2\theta$
T _{measurement} :	293 K
2 θ _{max} :	55°
N(hkl) _{unique} :	474
Criterion for F _o :	F _o > 4 σ (F _o)
N(param) _{refined} :	39
Program:	SHELXTL-plus

Source of material: The material was found on a brick of the oven covering on the area of the VDM Kupferwerk Heddernheim (see ref. 1).

The structure described by ref. 2 has been confirmed. Like other sheet silicates - $\text{BaCuSi}_4\text{O}_{10}$ (see refs. 5 and 6) and gillespite $\text{BaFeSi}_4\text{O}_{10}$ (see refs. 3 and 4) $\text{CaCuSi}_4\text{O}_{10}$ has an almost straight $\text{Si}-\text{O}-\text{Si}$ bond (177.2°) in addition to the normal ones (149.0°). The Cu atoms are in a square planar environment of four O atoms. The Ca atoms are coordinated by eight O atoms.

CaCuSi₄O₁₀, tetragonal, *P4/ncc* (No. 130), *a* = 7.314(1) Å, *c* = 15.168(8) Å, *V* = 811.4 Å³, *Z* = 4, *R*(*F*) = 0.017, *R*_w(*F*) = 0.021.

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}
Cu	4c	0	1/2	0.08174(3)	0.0049(2)	0.0049(2)	0.0112(3)	0	0	0
Ca	4b	0	0	0	0.0086(3)	0.0086(3)	0.0088(4)	0	0	0
Si	16g	0.25297(6)	0.17687(6)	0.14739(3)	0.0052(3)	0.0055(3)	0.0080(3)	0.0000(2)	0.0005(2)	-0.0006(2)
O(1)	8f	0.2112(2)	x	1/4	0.0241(6)	0.0241(6)	0.0108(9)	-0.0034(8)	0.2173(6)	-0.0056(6)
O(2)	16g	0.4575(2)	0.2520(2)	0.12642(8)	0.0066(5)	0.0149(6)	0.0161(6)	-0.0016(5)	-0.0012(5)	0.0027(4)
O(3)	16g	0.1032(2)	0.2573(1)	0.08213(8)	0.0083(6)	0.0067(6)	0.0174(7)	0.0015(4)	-0.0037(4)	-0.0011(4)

References

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