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$CaCu_{1.424}Fe_{0.576}Si_2$

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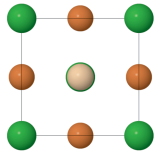
Structural data: full structural data are available from iucrdata.iucr.org

A $CaCu_{1.424}Fe_{0.576}Si_2$ phase was obtained during high-pressure sintering of an Si-rich quasicrystal composition prealloy with the nominal chemical composition $Si_{61}Cu_{30}Ca_7Fe_2$. The obtained phase crystallizes in the space group *I*4/*mmm* (No. 139), with $a = b = 4.041$ Å and $c = 10.010$ Å. It is isotypic with $CaCu_2Si_2$ ($a = b =$ 4.06 Å and $c = 9.91$ Å) [Palenzona *et al.* (1986). *J. Less-Common Met.* **119**, 199–209] and $CaFe_2Si_2$ ($a = b = 3.94$ Å and $c = 10.19$ Å) [Hlukhyy *et al.* (2012). *Z. Anorg. Allg. Chem.* **638**, 1619–1619]. It features a co-occupancy of Cu and Fe atoms with a ratio of the refined site-occupancy factors of 0.71 (15):0.29 (15).

3D view



Structure description

It has been reported that Si-rich quasicrystals form under extreme conditions during atomic bomb explosion (Bindi *et al.*, 2021). In this work, we took the Si-rich quasicrystal compostion and applied our high-pressure sintering methodology to reveal phases forming at this composition in a laboratory experiment and obtained crystals of the composition $CaCu_{1.424}Fe_{0.576}Si_2$. This phase shows remarkable structural similarities to $BaFe_{1.8}Co_{0.2}As_2$ ($a = b = 3.96$ Å and $c = 13.96$ Å) reported by Sefat *et al.* (2008), sharing identical space-group symmetry and analogous co-site-occupation behaviour. $CaCu_{1.424}Fe_{0.576}Si_2$, as well as $BaFe_{1.8}Co_{0.2}As_2$, and along with other AETX-type compounds (AE = alkaline earth metals, T = transition metals and X = Si, Ge, As), belong to the 122-type structure and all show the space group *I*4/*mmm*.

The distribution of atoms in the crystal unit of $CaCu_{1.424}Fe_{0.576}Si_2$ is illustrated in Fig. 1. The coordination environment of the Ca atom is shown in Fig. 2. The Ca1 atom is located in a position with 4/*mmm* symmetry (multiplicity 2, Wyckoff symbol *a*). It is surrounded by eight Si1 atoms (4*mm*, 4 *e*) and eight Cu1/Fe1 atoms ($\bar{4}m2$, 4 *d*), forming the centre of a

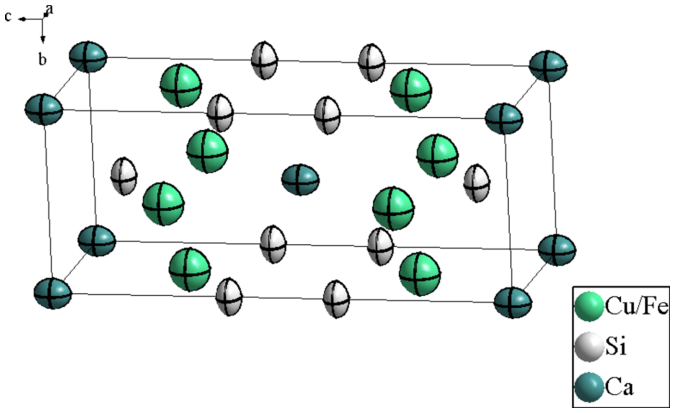


Figure 1
The crystal structure of $CaCu_{1.424}Fe_{0.576}Si_2$ (one unit cell), with displacement ellipsoids drawn at the 99% probability level.

tetradecahedron. The shortest distance between calcium and silicon is Ca1—Si1 = 3.087 (4) Å, whereas the longest Ca1—Cu1/Fe1 bond is 3.216 (2) Å.

This study refined the crystal structure model of $CaCu_{1.424}Fe_{0.576}Si_2$based on single-crystal X-ray diffraction data. Its composition was confirmed by EDX results.

Synthesis and crystallization

High-purity elements Ca (99.5% purity, 0.068 g), Cu (99.5% purity, 0.4718 g), Fe (99.9% purity, 0.0247 g) and Si (99.5% purity, 0.4270 g) were weighed precisely according to a stoichiometric ratio of 7:30:2:61. The mixture was homogenized and thoroughly ground in an agate mortar. Subsequently, the blended powder was loaded into a tungsten carbide die with a 5 mm inner diameter and compacted at 6 MPa for 3 min to form cylindrical pellets. These pellets were subjected to high-pressure sintering experiments using a six-anvil apparatus (Liu & Fan, 2018), where samples were pressurized to 6 GPa and heated to 1573 K for 40 min, followed by rapid quenching to room temperature through furnace power termination. A regular specimen was selected and mounted on a glass fiber using adhesive for X-ray diffraction measurements.

Table 1
Experimental details.

Crystal data	
Chemical formula	$CaCu_{1.42}Fe_{0.58}Si_2$
M_r	218.91
Crystal system, space group	Tetragonal, *I*4/*mmm*
Temperature (K)	296
a, *c* (Å)	4.041 (3), 10.010 (9)
V (Å^3)	163.5 (3)
Z	2
Radiation type	Mo *Kα*
μ (mm^{-1})	13.82
Crystal size (mm)	0.10 × 0.07 × 0.06
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.383, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	707, 60, 46
R_{int}	0.097
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.588
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.071, 0.156, 1.29
No. of reflections	60
No. of parameters	9
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.05, −1.45

Computer programs: *APEX5* (Bruker, 2023), *SAINT* (Bruker, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2017) and *publCIF* (Westrip, 2010).

Refinement

Comprehensive crystallographic data, data collection parameters and structure refinement details are summarized in

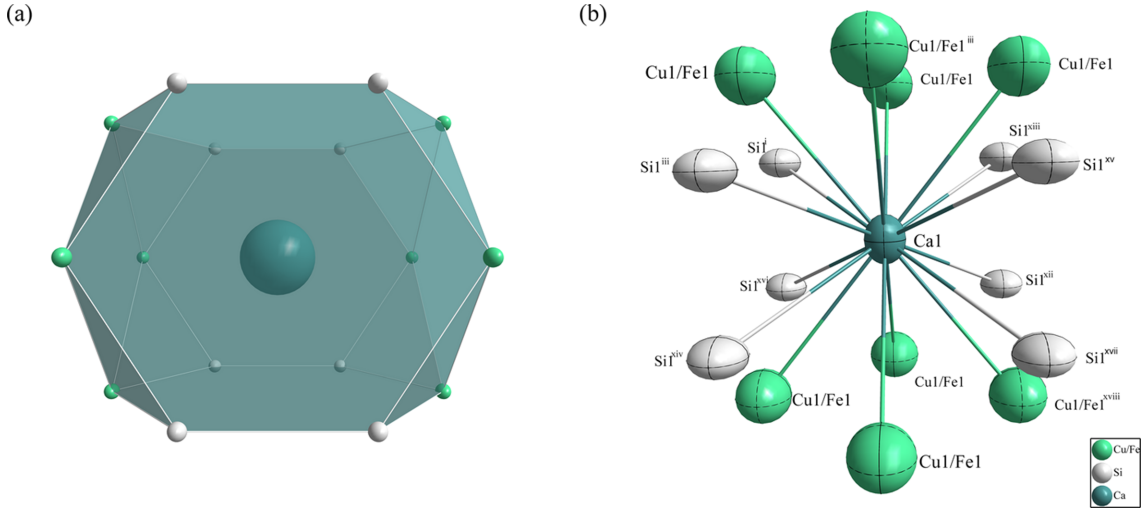


Figure 2
(*a*) The tetradecahedron formed around the Ca1 atom at the 2 *a* site and (*b*) the environment of the Ca1 atom, with displacement ellipsoids given at the 99% probability level. [Symmetry codes: (i) $-x-\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$; (xii) $x-\frac{1}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (xiii) $-x-\frac{1}{2}, -y-\frac{1}{2}, -z+\frac{1}{2}$; (xiv) $x+\frac{1}{2}, y+\frac{1}{2}, z-\frac{1}{2}$; (xv) $-x+\frac{1}{2}, -y-\frac{1}{2}, -z+\frac{1}{2}$; (xvi) $x-\frac{1}{2}, y+\frac{1}{2}, z-\frac{1}{2}$; (xvii) $x+\frac{1}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (xviii) $-x, -y, -z$.]

Table 1. To facilitate comparative analysis, the labelling scheme and atomic coordinates for $CaCu_{1.424}Fe_{0.576}Si_2$ were taken from the corresponding data of $CaCu_2Si_2$ (Palenzona *et al.*, 1986) and $CaFe_2Si_2$ (Hlukhyy *et al.*, 2012). The sites of the occupancy factors for the co-occupancy of the Cu and Fe atoms refined to 0.71 (15) and 0.29 (15), respectively. The command 'SHEL 999 0.84' was used to eliminate weakly diffracting high-angle data. The maximum and minimum residual electron densities in the final difference map are located at 0.99 Å from Ca1 and 0.00 Å from Cu1, respectively.

Funding information

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full crystallographic data

IUCrData (2025). **10**, x250325 [https://doi.org/10.1107/S2414314625003256]

$CaCu_{1.424}Fe_{0.576}Si_2$

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Calcium copper iron disilicide

Crystal data

$CaCu_{1.42}Fe_{0.58}Si_2$
M_r = 218.91
Tetragonal, *I*4/*mmm*
a = 4.041 (3) Å
c = 10.010 (9) Å
V = 163.5 (3) Å^3
Z = 2
F(000) = 209
D_x = 4.448 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 452 reflections
θ = 4.1–26.9°
μ = 13.82 mm^{-1}
T = 296 K
Lump, gray
0.10 × 0.07 × 0.06 mm

Data collection

Bruker D8 Venture Photon 100 CMOS diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.383, T_{max} = 0.746
707 measured reflections
60 independent reflections
46 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
θ_{max} = 24.7°, θ_{min} = 4.1°
h = −4→4
k = −4→4
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.156
S = 1.29
60 reflections
9 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0957P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −1.45 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Fe1	0.000000	0.500000	0.250000	0.0171 (18)	0.29 (15)
Cu1	0.000000	0.500000	0.250000	0.0171 (18)	0.71 (15)

Si1	0.000000	0.000000	0.3834 (10)	0.011 (3)
Ca1	0.000000	0.000000	0.000000	0.011 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0178 (19)	0.0178 (19)	0.016 (3)	0.000	0.000	0.000
Cu1	0.0178 (19)	0.0178 (19)	0.016 (3)	0.000	0.000	0.000
Si1	0.013 (4)	0.013 (4)	0.006 (7)	0.000	0.000	0.000
Ca1	0.009 (4)	0.009 (4)	0.013 (7)	0.000	0.000	0.000

Geometric parameters (Å, º)

Fe1—Si1	2.422 (6)	Cu1—Si1^{i}	2.422 (6)
Fe1—Si1^{i}	2.422 (6)	Cu1—Si1^{ii}	2.422 (6)
Fe1—Si1^{ii}	2.422 (6)	Cu1—Si1^{iii}	2.422 (6)
Fe1—Si1^{iii}	2.422 (6)	Cu1—Ca1^{vi}	3.216 (2)
Fe1—Fe1^{i}	2.857 (2)	Cu1—Ca1	3.216 (2)
Fe1—Fe1^{iv}	2.857 (2)	Cu1—Ca1^{ii}	3.216 (2)
Fe1—Fe1^{iii}	2.857 (2)	Cu1—Ca1^{vii}	3.216 (2)
Fe1—Fe1^{v}	2.857 (2)	Si1—Si1^{viii}	2.33 (2)
Fe1—Ca1^{vi}	3.216 (2)	Si1—Ca1^{vi}	3.087 (4)
Fe1—Ca1	3.216 (2)	Si1—Ca1^{ix}	3.087 (4)
Fe1—Ca1^{ii}	3.216 (2)	Si1—Ca1^{x}	3.087 (4)
Fe1—Ca1^{vii}	3.216 (2)	Si1—Ca1^{vii}	3.087 (4)
Cu1—Si1	2.422 (6)		
Si1—Fe1—Si1^{i}	107.7 (2)	Fe1^{i}—Si1—Fe1	72.3 (2)
Si1—Fe1—Si1^{ii}	113.1 (4)	Fe1^{xi}—Si1—Fe1	113.1 (4)
Si1^{i}—Fe1—Si1^{ii}	107.7 (2)	Si1^{viii}—Si1—Cu1	123.5 (2)
Si1—Fe1—Si1^{iii}	107.7 (2)	Si1^{viii}—Si1—Fe1^{iii}	123.5 (2)
Si1^{i}—Fe1—Si1^{iii}	113.1 (4)	Fe1^{i}—Si1—Fe1^{iii}	113.1 (4)
Si1^{ii}—Fe1—Si1^{iii}	107.7 (2)	Fe1^{xi}—Si1—Fe1^{iii}	72.3 (2)
Si1—Fe1—Fe1^{i}	53.85 (10)	Fe1—Si1—Fe1^{iii}	72.3 (2)
Si1^{i}—Fe1—Fe1^{i}	53.85 (10)	Si1^{viii}—Si1—Ca1^{vi}	67.78 (18)
Si1^{ii}—Fe1—Fe1^{i}	126.15 (10)	Fe1^{i}—Si1—Ca1^{vi}	138.99 (9)
Si1^{iii}—Fe1—Fe1^{i}	126.15 (10)	Fe1^{xi}—Si1—Ca1^{vi}	138.99 (9)
Si1—Fe1—Fe1^{iv}	126.15 (10)	Fe1—Si1—Ca1^{vi}	70.27 (4)
Si1^{i}—Fe1—Fe1^{iv}	126.15 (10)	Cu1—Si1—Ca1^{vi}	70.27 (4)
Si1^{ii}—Fe1—Fe1^{iv}	53.85 (10)	Fe1^{iii}—Si1—Ca1^{vi}	70.27 (4)
Si1^{iii}—Fe1—Fe1^{iv}	53.85 (10)	Si1^{viii}—Si1—Ca1^{ix}	67.78 (18)
Fe1^{i}—Fe1—Fe1^{iv}	180.0	Fe1^{i}—Si1—Ca1^{ix}	70.27 (4)
Si1—Fe1—Fe1^{iii}	53.85 (10)	Fe1^{xi}—Si1—Ca1^{ix}	70.27 (4)
Si1^{i}—Fe1—Fe1^{iii}	126.15 (10)	Fe1—Si1—Ca1^{ix}	138.99 (9)
Si1^{ii}—Fe1—Fe1^{iii}	126.15 (10)	Fe1^{iii}—Si1—Ca1^{ix}	138.99 (9)
Si1^{iii}—Fe1—Fe1^{iii}	53.85 (10)	Ca1^{vi}—Si1—Ca1^{ix}	135.6 (4)
Fe1^{i}—Fe1—Fe1^{iii}	90.0	Si1^{viii}—Si1—Ca1^{x}	67.78 (18)
Fe1^{iv}—Fe1—Fe1^{iii}	90.0	Fe1^{i}—Si1—Ca1^{x}	138.99 (9)

Si1—Fe1—Fe1^{v}	126.15 (10)	Fe1^{xi}—Si1—Ca1^{x}	70.27 (4)
Si1^{i}—Fe1—Fe1^{v}	53.85 (10)	Fe1—Si1—Ca1^{x}	138.99 (9)
Si1^{ii}—Fe1—Fe1^{v}	53.85 (10)	Fe1^{iii}—Si1—Ca1^{x}	70.27 (4)
Si1^{iii}—Fe1—Fe1^{v}	126.15 (10)	Ca1^{vi}—Si1—Ca1^{x}	81.78 (13)
Fe1^{i}—Fe1—Fe1^{v}	90.0	Ca1^{ix}—Si1—Ca1^{x}	81.78 (13)
Fe1^{iv}—Fe1—Fe1^{v}	90.0	Si1^{viii}—Si1—Ca1^{vii}	67.78 (18)
Fe1^{iii}—Fe1—Fe1^{v}	180.0	Fe1^{i}—Si1—Ca1^{vii}	70.27 (4)
Si1—Fe1—Ca1^{vi}	64.60 (15)	Fe1^{xi}—Si1—Ca1^{vii}	138.99 (9)
Si1^{i}—Fe1—Ca1^{vi}	162.4 (2)	Fe1—Si1—Ca1^{vii}	70.27 (4)
Si1^{ii}—Fe1—Ca1^{vi}	64.60 (15)	Fe1^{iii}—Si1—Ca1^{vii}	138.99 (9)
Si1^{iii}—Fe1—Ca1^{vi}	84.5 (2)	Ca1^{vi}—Si1—Ca1^{vii}	81.78 (13)
Fe1^{i}—Fe1—Ca1^{vi}	116.37 (2)	Ca1^{ix}—Si1—Ca1^{vii}	81.78 (13)
Fe1^{iv}—Fe1—Ca1^{vi}	63.628 (19)	Ca1^{x}—Si1—Ca1^{vii}	135.6 (4)
Fe1^{iii}—Fe1—Ca1^{vi}	63.63 (2)	Si1^{iii}—Ca1—Si1^{xii}	180.0
Fe1^{v}—Fe1—Ca1^{vi}	116.37 (2)	Si1^{iii}—Ca1—Si1^{xiii}	135.6 (4)
Si1—Fe1—Ca1	84.5 (2)	Si1^{xii}—Ca1—Si1^{xiii}	44.4 (4)
Si1^{i}—Fe1—Ca1	64.60 (15)	Si1^{iii}—Ca1—Si1^{xiv}	44.4 (4)
Si1^{ii}—Fe1—Ca1	162.4 (2)	Si1^{xii}—Ca1—Si1^{xiv}	135.6 (4)
Si1^{iii}—Fe1—Ca1	64.60 (15)	Si1^{xiii}—Ca1—Si1^{xiv}	180.0
Fe1^{i}—Fe1—Ca1	63.63 (2)	Si1^{iii}—Ca1—Si1^{i}	81.78 (13)
Fe1^{iv}—Fe1—Ca1	116.37 (2)	Si1^{xii}—Ca1—Si1^{i}	98.22 (13)
Fe1^{iii}—Fe1—Ca1	63.63 (2)	Si1^{xiii}—Ca1—Si1^{i}	81.78 (13)
Fe1^{v}—Fe1—Ca1	116.37 (2)	Si1^{xiv}—Ca1—Si1^{i}	98.22 (13)
Ca1^{vi}—Fe1—Ca1	127.26 (4)	Si1^{iii}—Ca1—Si1^{xv}	81.78 (13)
Si1—Fe1—Ca1^{ii}	162.4 (2)	Si1^{xii}—Ca1—Si1^{xv}	98.22 (13)
Si1^{i}—Fe1—Ca1^{ii}	64.60 (15)	Si1^{xiii}—Ca1—Si1^{xv}	81.78 (13)
Si1^{ii}—Fe1—Ca1^{ii}	84.5 (2)	Si1^{xiv}—Ca1—Si1^{xv}	98.22 (13)
Si1^{iii}—Fe1—Ca1^{ii}	64.60 (15)	Si1^{i}—Ca1—Si1^{xv}	135.6 (4)
Fe1^{i}—Fe1—Ca1^{ii}	116.37 (2)	Si1^{iii}—Ca1—Si1^{xvi}	98.22 (13)
Fe1^{iv}—Fe1—Ca1^{ii}	63.63 (2)	Si1^{xii}—Ca1—Si1^{xvi}	81.78 (13)
Fe1^{iii}—Fe1—Ca1^{ii}	116.37 (2)	Si1^{xiii}—Ca1—Si1^{xvi}	98.22 (13)
Fe1^{v}—Fe1—Ca1^{ii}	63.63 (2)	Si1^{xiv}—Ca1—Si1^{xvi}	81.78 (13)
Ca1^{vi}—Fe1—Ca1^{ii}	127.26 (4)	Si1^{i}—Ca1—Si1^{xvi}	44.4 (4)
Ca1—Fe1—Ca1^{ii}	77.83 (7)	Si1^{xv}—Ca1—Si1^{xvi}	180.0
Si1—Fe1—Ca1^{vii}	64.60 (15)	Si1^{iii}—Ca1—Si1^{xvii}	98.22 (13)
Si1^{i}—Fe1—Ca1^{vii}	84.5 (2)	Si1^{xii}—Ca1—Si1^{xvii}	81.78 (13)
Si1^{ii}—Fe1—Ca1^{vii}	64.60 (15)	Si1^{xiii}—Ca1—Si1^{xvii}	98.22 (13)
Si1^{iii}—Fe1—Ca1^{vii}	162.4 (2)	Si1^{xiv}—Ca1—Si1^{xvii}	81.78 (13)
Fe1^{i}—Fe1—Ca1^{vii}	63.63 (2)	Si1^{i}—Ca1—Si1^{xvii}	180.0
Fe1^{iv}—Fe1—Ca1^{vii}	116.37 (2)	Si1^{xv}—Ca1—Si1^{xvii}	44.4 (4)
Fe1^{iii}—Fe1—Ca1^{vii}	116.37 (2)	Si1^{xvi}—Ca1—Si1^{xvii}	135.6 (4)
Fe1^{v}—Fe1—Ca1^{vii}	63.63 (2)	Si1^{iii}—Ca1—Fe1	45.14 (14)
Ca1^{vi}—Fe1—Ca1^{vii}	77.83 (7)	Si1^{xii}—Ca1—Fe1	134.86 (14)
Ca1—Fe1—Ca1^{vii}	127.26 (4)	Si1^{xiii}—Ca1—Fe1	96.72 (17)
Ca1^{ii}—Fe1—Ca1^{vii}	127.26 (4)	Si1^{xiv}—Ca1—Fe1	83.28 (17)
Si1—Cu1—Si1^{i}	107.7 (2)	Si1^{i}—Ca1—Fe1	45.14 (14)
Si1—Cu1—Si1^{ii}	113.1 (4)	Si1^{xv}—Ca1—Fe1	96.72 (17)
Si1^{i}—Cu1—Si1^{ii}	107.7 (2)	Si1^{xvi}—Ca1—Fe1	83.28 (17)

Si1—Cu1—Si1^{iii}	107.7 (2)	Si1^{xvii}—Ca1—Fe1	134.86 (14)
Si1^{i}—Cu1—Si1^{iii}	113.1 (4)	Si1^{iii}—Ca1—Fe1^{iii}	45.14 (14)
Si1^{ii}—Cu1—Si1^{iii}	107.7 (2)	Si1^{xii}—Ca1—Fe1^{iii}	134.86 (14)
Si1—Cu1—Ca1^{vi}	64.60 (15)	Si1^{xiii}—Ca1—Fe1^{iii}	96.72 (17)
Si1^{i}—Cu1—Ca1^{vi}	162.4 (2)	Si1^{xiv}—Ca1—Fe1^{iii}	83.28 (17)
Si1^{ii}—Cu1—Ca1^{vi}	64.60 (15)	Si1^{i}—Ca1—Fe1^{iii}	96.72 (17)
Si1^{iii}—Cu1—Ca1^{vi}	84.5 (2)	Si1^{xv}—Ca1—Fe1^{iii}	45.14 (14)
Si1—Cu1—Ca1	84.5 (2)	Si1^{xvi}—Ca1—Fe1^{iii}	134.86 (14)
Si1^{i}—Cu1—Ca1	64.60 (15)	Si1^{xvii}—Ca1—Fe1^{iii}	83.28 (17)
Si1^{ii}—Cu1—Ca1	162.4 (2)	Fe1—Ca1—Fe1^{iii}	52.74 (4)
Si1^{iii}—Cu1—Ca1	64.60 (15)	Si1^{iii}—Ca1—Cu1	45.14 (14)
Ca1^{vi}—Cu1—Ca1	127.26 (4)	Si1^{xii}—Ca1—Cu1	134.86 (14)
Si1—Cu1—Ca1^{ii}	162.4 (2)	Si1^{xiii}—Ca1—Cu1	96.72 (17)
Si1^{i}—Cu1—Ca1^{ii}	64.60 (15)	Si1^{xiv}—Ca1—Cu1	83.28 (17)
Si1^{ii}—Cu1—Ca1^{ii}	84.5 (2)	Si1^{i}—Ca1—Cu1	45.14 (14)
Si1^{iii}—Cu1—Ca1^{ii}	64.60 (15)	Si1^{xv}—Ca1—Cu1	96.72 (17)
Ca1^{vi}—Cu1—Ca1^{ii}	127.26 (4)	Si1^{xvi}—Ca1—Cu1	83.28 (17)
Ca1—Cu1—Ca1^{ii}	77.83 (7)	Si1^{xvii}—Ca1—Cu1	134.86 (14)
Si1—Cu1—Ca1^{vii}	64.60 (15)	Si1^{iii}—Ca1—Fe1^{xviii}	134.86 (14)
Si1^{i}—Cu1—Ca1^{vii}	84.5 (2)	Si1^{xii}—Ca1—Fe1^{xviii}	45.14 (14)
Si1^{ii}—Cu1—Ca1^{vii}	64.60 (15)	Si1^{xiii}—Ca1—Fe1^{xviii}	83.28 (17)
Si1^{iii}—Cu1—Ca1^{vii}	162.4 (2)	Si1^{xiv}—Ca1—Fe1^{xviii}	96.72 (17)
Ca1^{vi}—Cu1—Ca1^{vii}	77.83 (7)	Si1^{i}—Ca1—Fe1^{xviii}	134.86 (14)
Ca1—Cu1—Ca1^{vii}	127.26 (4)	Si1^{xv}—Ca1—Fe1^{xviii}	83.28 (17)
Ca1^{ii}—Cu1—Ca1^{vii}	127.26 (4)	Si1^{xvi}—Ca1—Fe1^{xviii}	96.72 (17)
Si1^{viii}—Si1—Fe1^{i}	123.5 (2)	Si1^{xvii}—Ca1—Fe1^{xviii}	45.14 (14)
Si1^{viii}—Si1—Fe1^{xi}	123.5 (2)	Fe1—Ca1—Fe1^{xviii}	180.0
Fe1^{i}—Si1—Fe1^{xi}	72.3 (2)	Fe1^{iii}—Ca1—Fe1^{xviii}	127.26 (4)
Si1^{viii}—Si1—Fe1	123.5 (2)		

Symmetry codes: (i) $-x-1/2, -y+1/2, -z+1/2$; (ii) $x, y+1, z$; (iii) $-x+1/2, -y+1/2, -z+1/2$; (iv) $-x+1/2, -y+3/2, -z+1/2$; (v) $-x-1/2, -y+3/2, -z+1/2$; (vi) $x+1/2, y+1/2, z+1/2$; (vii) $x-1/2, y+1/2, z+1/2$; (viii) $-x, -y, -z+1$; (ix) $x-1/2, y-1/2, z+1/2$; (x) $x+1/2, y-1/2, z+1/2$; (xi) $x, y-1, z$; (xii) $x-1/2, y-1/2, z-1/2$; (xiii) $-x-1/2, -y-1/2, -z+1/2$; (xiv) $x+1/2, y+1/2, z-1/2$; (xv) $-x+1/2, -y-1/2, -z+1/2$; (xvi) $x-1/2, y+1/2, z-1/2$; (xvii) $x+1/2, y-1/2, z-1/2$; (xviii) $-x, -y, -z$.