Crystal structure of calcium iron zinc *catena*-disilicate, $Ca(Fe_{0.19}Zn_{0.81})Si_2O_6$

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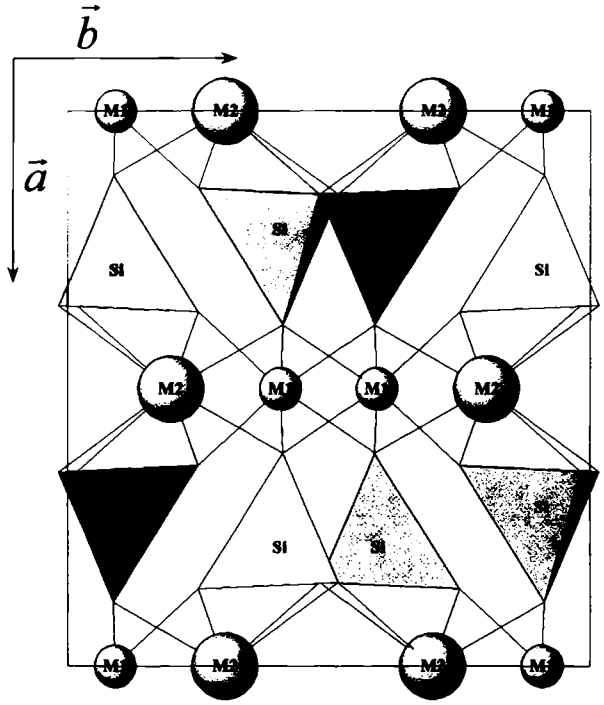

Abstract

$CaFe_{0.19}O_6Si_2Zn_{0.81}$, monoclinic, *C*12/*c*1 (No. 15), $a = 9.8093(7)$ Å, $b = 8.9817(7)$ Å, $c = 5.2527(4)$ Å, $\beta = 105.66(1)°$, $V = 445.6$ Å^3, $Z = 4$, $R_{gt(F)} = 0.025$, $wR_{ref(F^2)} = 0.061$, $T = 293$ K.

Source of material

Single crystals of $Ca_{1.00(1)}Fe_{0.21(2)}Zn_{0.85(3)}Si_{1.97(1)}O_6$ were obtained under high pressure and high temperature conditions. Starting with a stoichiometric mixture of oxides (purity > 99.999%) the synthesis was performed in a Piston-Cylinder apparatus over 3 days with a temperature of 1473 K and a pressure of 2.5 GPa. The chemical composition of the crystal was determined by electron microprobe (CAMECA SX50, 15 kV/15 nA, standards: wollastonite $CaSiO_3$, hematite Fe_2O_3, and sphalerite ZnS).

Discussion

The investigated material has a clinopyroxene structure [1] in which Zn^{2+} shares the M1 position with Fe^{2+}. The M2-site is completely occupied by Ca^{2+}. In the most structures zinc is tetrahedral coordinated [2,3] and the octahedral coordination of zinc in pyroxenes is an exception. This is also expressed in the distortion of the Zn-containing M2-site. Comparing to $CaFeSi_2O_6$ we find shorter *d*(M1—O2) (2.0733(9) Å) and *d*(M1—O1) (2.0849(9) Å) distances but no changes in the M1—O1 length (2.1595(9) Å). The lattice parameters of the material were determined by powder diffraction.

Table 1. Data collection and handling.

Crystal:	light yellow fragment, size 0.16 × 0.19 × 0.290 mm
Wavelength:	Mo K_α radiation (0.70932 Å)
μ:	69.7 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{max}$:	80.02°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1706, 1389
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1299
$N(param)_{refined}$:	50
Program:	SHELXL-97 [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(M1)	4*e*	0.810(1)	0	0.90590(2)	1/4	0.0123(1)	0.0119(1)	0.0106(1)	0	0.00289(7)	0
Fe(M1)	4*e*	0.190	0	0.90590	1/4	0.0123	0.0119	0.0106	0	0.00289	0
Ca(M2)	4*e*		0	0.30017(4)	1/4	0.0156(1)	0.0128(1)	0.0120(1)	0	0.0015(1)	0
Si(T1)	8*f*		0.28672(4)	0.09259(3)	0.22966(7)	0.0101(2)	0.0104(2)	0.0097(1)	-0.00022(8)	0.0030(1)	-0.00025(8)
O(1)	8*f*		0.1169(1)	0.08914(9)	0.1455(2)	0.0106(3)	0.0134(3)	0.0118(3)	0.0005(2)	0.0028(3)	0.0003(2)
O(2)	8*f*		0.3607(1)	0.2480(1)	0.3218(2)	0.0152(3)	0.0118(3)	0.0137(3)	-0.0025(3)	0.0037(3)	-0.0006(3)
O(3)	8*f*		0.35019(8)	0.0190(1)	0.9939(2)	0.0123(3)	0.0144(3)	0.0112(3)	-0.0002(2)	0.0038(3)	-0.0026(2)

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