Crystal structure of calcium iron zinc *catena*-disilicate, $Ca(Fe_{0.52}Zn_{0.48})Si_2O_6$

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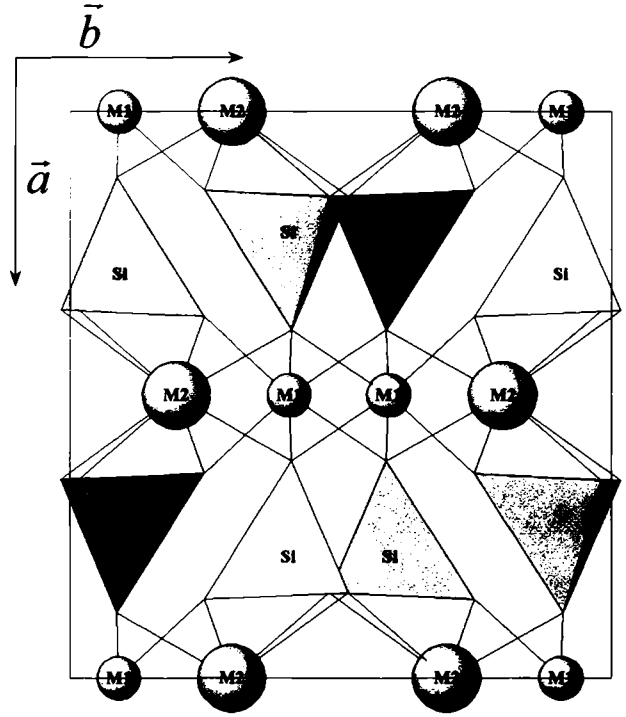

Abstract

$CaFe_{0.52}O_6Si_2Zn_{0.48}$, monoclinic, $C12/c1$ (No. 15), $a = 9.8206(8)$ Å, $b = 8.9966(8)$ Å, $c = 5.2487(4)$ Å, $\beta = 105.34(1)°$, $V = 447.2$ Å^3, $Z = 4$, $R_{gt}(F) = 0.029$, $wR_{ref}(F^2) = 0.067$, $T = 293$ K.

Source of material

Single crystals of $Ca_{0.98(2)}Fe_{0.59(3)}Zn_{0.46(3)}Si_{1.98(2)}O_6$ 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 65 hours with a temperature of 1123 K and a pressure of 1.8 GPa. The chemical composition of the crystal was determined by electron microprobe (CAMECA SX50, 15 kV/20 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 tetrahedrally 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) (2.077(1) Å) and d(M1—O1) (2.103(1) Å) distances but no changes in the M1—O1 length (2.160(1) Å). The lattice parameters of the material were determined by powder diffraction.

Table 1. Data collection and handling.

Crystal:	yellow fragment, size 0.053 × 0.213 × 0.213 mm
Wavelength:	Mo K_α radiation (0.70932 Å)
μ:	60.6 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{max}$:	80.06°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1718, 1396
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1222
$N(param)_{refined}$:	49
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*	0.483(9)	0	0.90635(3)	1/4	0.0101(1)	0.0086(1)	0.0083(1)	0	0.00229(8)	0
Fe(M1)	4*e*	0.517	0	0.90635	1/4	0.0101	0.0086	0.0083	0	0.00229	0
Ca(M2)	4*e*		0	0.30019(4)	1/4	0.0140(2)	0.0098(1)	0.0098(1)	0	0.0011(1)	0
Si(T1)	8*f*		0.28709(4)	0.09252(4)	0.23072(7)	0.0084(2)	0.0075(2)	0.0074(2)	–0.0003(1)	0.0023(1)	–0.00025(9)
O(1)	8*f*		0.1178(1)	0.0894(1)	0.1479(2)	0.0083(4)	0.0103(4)	0.0101(4)	0.0002(3)	0.0023(3)	0.0004(3)
O(2)	8*f*		0.3615(1)	0.2473(1)	0.3223(2)	0.0141(4)	0.0088(4)	0.0120(3)	–0.0030(3)	0.0035(3)	–0.0008(3)
O(3)	8*f*		0.3502(1)	0.0190(1)	0.9932(2)	0.0101(4)	0.0121(4)	0.0091(3)	–0.0002(3)	0.0029(3)	–0.0025(3)

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