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Thermal behaviour
of the crystal structure of strontian piemontite

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Abstract

Unit-cell constants of a strontian-piemontite sample from S. Marcel (Val d'Aosta, Italy) with composition $\text{Ca}_{1.00}\text{Sr}_{0.00}\text{Al}_{1.00}\text{Fe}_{0.00}\text{Mn}_{0.00}\text{Si}_2\text{O}_{12}\text{OH}$ were measured at several temperatures by single-crystal X-ray diffractometry (MoK α radiation). Values at 25 and 800°C were $a = 8.884(3)$, $b = 5.684(1)$, $c = 10.202(3)\text{\AA}$, $\beta = 115.23(2)^\circ$; and $a = 8.934(9)$, $b = 5.727(4)$, $c = 10.30(1)\text{\AA}$, $\beta = 115.26(9)^\circ$, respectively; space group $P2_1/m$; principal coefficients of thermal expansion 0.72, 0.98 and $1.29 \times 10^{-5}\text{K}^{-1}$. Sets of 3385 and 2180 independent intensity data were measured at 25 and 800°C, respectively, and the corresponding least-squares refinements of the crystal structure converged to $R = 0.041$ and 0.056. The thermal-expansion ellipsoid is symmetrically oriented with respect to a and c . A significant shrinking of the Si_2O_7 group, with opening of the Si-O-Si angle, is observed at high temperature. A large and very anisotropic mean expansion ($1.4 \times 10^{-5}\text{K}^{-1}$) occurs for the (Mn,Fe) coordination octahedron [M(3) site]. The relation between thermal expansion of the lattice and of coordination polyhedra is accounted for by a correlated tilting of polyhedra at high temperature. No deprotonation can be detected before the breakdown of the structure (880°C); the dehydration products have been identified.

Anisotropic thermal parameters $B_{i,j}$ (\AA^2) for piemontite at 25 (upper) and 800°C (lower) of the expression $\Sigma \Sigma \exp[-(1/4)(B_{i,j} h_i h_j a^{*i} a^{*j})]$. Esd's are in parentheses.

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
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A(1)	1.04(2) 2.85(5)	0.78(1) 2.24(5)	0.78(1) 2.26(3)	— —	0.59(1) 1.75(3)	— —
A(2)	0.88(1) 2.22(3)	1.33(1) 3.87(5)	0.56(1) 1.74(3)	— —	0.22(9) 0.78(3)	— —
M(1)	0.42(2) 1.12(3)	0.42(2) 1.12(4)	0.50(2) 1.32(3)	-0.02(1) -0.13(4)	0.16(1) 0.51(3)	0.02(1) -0.11(4)
M(2)	0.40(2) 1.15(5)	0.41(2) 1.18(5)	0.51(2) 1.46(3)	-0.03(2) -0.06(4)	0.18(2) 0.54(3)	-0.03(2) -0.02(4)
M(3)	0.37(1) 0.96(2)	0.56(1) 1.70(3)	0.53(1) 1.53(3)	— —	0.16(1) 0.50(2)	— —
Si(1)	0.49(2) 1.15(5)	0.53(2) 1.29(5)	0.51(2) 1.18(3)	— —	0.21(1) 0.60(3)	— —
Si(2)	0.45(2) 1.02(5)	0.55(2) 1.39(5)	0.53(2) 1.18(3)	— —	0.21(1) 0.54(3)	— —
Si(3)	0.47(2) 1.02(5)	0.57(2) 1.31(5)	0.54(2) 1.15(3)	— —	0.26(1) 0.60(3)	— —
O(1)	0.76(3) 1.72(8)	0.64(3) 2.1(1)	1.13(4) 2.7(1)	0.13(3) 0.31(9)	0.50(3) 1.26(9)	0.09(3) 0.4(1)
O(2)	0.71(3) 1.88(8)	0.76(4) 2.1(1)	0.80(3) 2.0(1)	-0.18(3) -0.52(9)	0.32(3) 0.90(9)	0.03(3) 0.02(9)
O(3)	0.54(3) 1.59(8)	0.63(4) 1.5(1)	0.86(3) 2.0(1)	0.07(3) 0.26(7)	-0.00(3) 0.24(9)	-0.06(3) -0.02(9)
O(4)	0.67(4) 1.3(1)	0.56(5) 1.8(1)	0.69(5) 1.2(1)	— —	0.32(4) 0.54(9)	— —
O(5)	0.57(4) 1.5(1)	0.90(5) 2.1(2)	0.60(5) 1.2(1)	— —	0.13(4) 0.51(9)	— —
O(6)	0.77(5) 1.9(1)	0.53(5) 1.8(1)	0.77(5) 1.9(1)	— —	0.48(4) 1.4(1)	— —
O(7)	0.68(5) 1.5(1)	1.02(6) 3.1(2)	0.76(5) 1.7(1)	— —	0.12(4) 0.2(1)	— —
O(8)	0.67(5) 1.3(1)	1.41(6) 4.0(2)	0.97(6) 2.7(2)	— —	0.47(4) 1.31(1)	— —

O(9)	1.48(6)	1.82(8)	0.71(6)	-	0.60(5)	-
	4.3(2)	5.0(3)	1.5(1)	-	1.7(2)	-
O(10)	0.67(4)	0.64(5)	0.69(5)	-	0.40(4)	-
	1.9(1)	1.1(1)	2.0(1)	-	1.3(1)	-

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
15	4	-1	5.7	5.9	15	5	-11	7.3	7.4	15	5	-10	17.9	19.0	15	5	-9	4.9	3.1
15	5	-7	7.7	8.5	15	5	-6	6.7	5.1	15	5	-5	19.1	20.0	15	5	-2	13.3	12.7
16	0	-14	7.3	7.9	16	0	-13	13.8	14.9	16	0	-12	10.7	10.7	16	0	-11	5.9	5.3
16	0	-9	7.8	8.0	16	0	-8	32.4	33.0	16	0	-7	6.5	6.9	16	0	-6	7.3	7.4
16	0	-3	7.5	8.7	16	0	-1	11.4	11.8	16	0	0	7.3	8.4	16	1	-14	7.3	7.3
16	1	-12	9.2	8.9	16	1	-11	5.7	5.6	16	1	-10	7.3	5.9	16	1	-9	5.6	3.3
16	1	-7	15.5	16.1	16	1	-5	20.7	20.5	16	1	-4	6.5	7.4	16	1	-2	8.9	9.4
16	2	-14	15.9	15.9	16	2	-13	14.4	14.5	16	2	-12	5.2	4.0	16	2	-11	6.0	4.7
16	2	-8	11.0	9.5	16	2	-7	20.0	19.3	16	2	-5	22.2	22.9	16	2	-3	9.7	9.9
16	3	-13	5.2	1.0	16	3	-12	8.5	7.7	16	3	-11	6.1	5.9	16	3	-10	7.2	6.7
16	3	-7	14.7	15.2	16	3	-5	17.8	18.1	16	3	-4	6.8	7.8	16	3	-2	9.1	9.3
16	4	-10	6.0	5.3	16	4	-9	6.2	7.2	16	4	-8	27.6	28.2	16	4	-7	7.2	6.9
16	4	-5	13.5	13.7	17	0	-13	14.1	14.7	17	0	-12	5.3	5.0	17	0	-11	23.7	24.4
17	0	-9	5.4	3.1	17	0	-8	5.6	4.5	17	0	-7	6.7	7.1	17	0	-6	9.7	9.2
17	0	-4	5.5	5.4	17	1	-13	13.3	13.7	17	1	-11	12.2	12.9	17	1	-10	16.8	18.3
17	1	-8	18.4	19.5	17	2	-12	5.3	4.4	17	2	-11	19.0	20.6	17	2	-10	5.9	6.7
17	2	-7	8.1	8.7	17	2	-6	6.2	6.2	17	2	-5	7.8	8.8	17	3	-9	9.7	8.8
															17	3	-8	18.8	19.6

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