Crystal structure of distrontium lithium magnesium trisilicide, $Sr_2(Li_xMg_{2-x})Si_3$ (x = 1)

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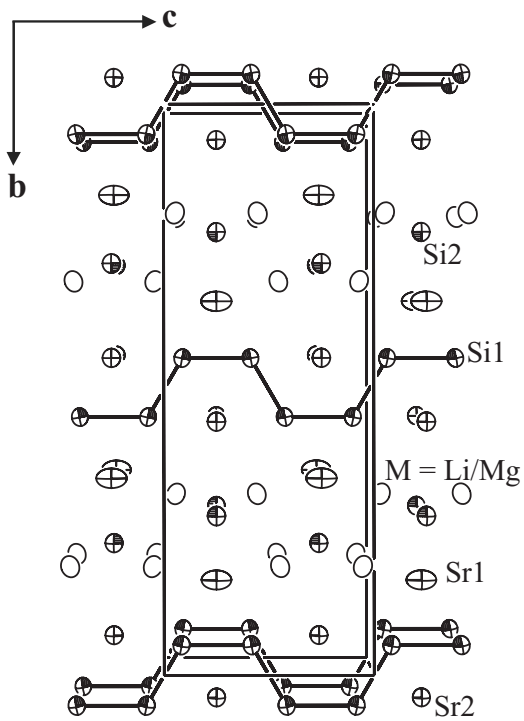

Abstract

$LiMgSi_3Sr_2$, orthorhombic, *Cmcm* (No. 63), a = 4.6179(5) Å, b = 19.488(2) Å, c = 7.1618(8) Å, V = 644.5 Å^3, Z = 4, $R_{gt}(F)$ = 0.029, $wR_{ref}(F^2)$ = 0.063, T = 293 K.

Source of material

$Sr_2LiMgSi_3$ was synthesized from a mixture of pure elements at stoichiometric amounts via direct heating in argon atmosphere up to 1123 K for 2h. After cooling down by a rate of 50 K/h, the product was obtained as dark grey crystals with metallic lustre.

Discussion

$Sr_2LiMgSi_3$ crystallizes in a layered structure similar to $EALiX_2$ (EA = Sr, Ba; X = Si, Ge) [1]. It contains one-dimensional Zintl anion chains in *cis-trans* conformation (Si—Si distance is 2.381(4) Å; the bond angle is 120.17(9)°). Every silicon atom on the chains is coordinated by a trigonal Sr_6 prism. In addition, there are also isolated Si^{4-} anions. It can be formulated as $(Sr^{2+})_2(Li^+)(Mg^{2+})(Si^{1.5-})_2(Si^{4-})$ according to the Zintl-Klemm concept [2-4]. Si^{4-} is also coordinated in a very typical way, situated at the centre of a trigonal Sr_5 bi-pyramid with all faces capped by M (M = Li, Mg) atoms. The structure relates also to the LaSi [5] structure type if a M_2Si unit is mitted. It can be considered as being isostructural to $Sr_2Mg_{(2-x)}Si_3$ [6]. However, it should be pointed out that the Sr1 site in the latter case is split into three positions (0 0.3495(4) 1/4; 0 0.3490(6) 0.2881(7); 0.065(1) 0.3371(3) 0.3236(8)), while it is well refined by one position here yet with a quite large displacement along c direction. This observation can be traced back to the irregular coordination sphere of Sr1. It is difficult to say if electronic factors might also play an important role. The M position is coordinated by a Si_4 tetrahedron, it is situated at the centre of a Sr_5 tetragonal pyramid.

Table 1. Data collection and handling.

Crystal:	dark grey plate, size 0.12 × 0.18 × 0.18 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	170.65 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, ω
$2\theta_{max}$:	67.66°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5018, 732
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 515
$N(param)_{refined}$:	26
Programs:	SHELXS-97 [7], SHELXL-97 [8], ORTEP-3 [9]

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sr(1)	4*c*	0	0.34517(3)	1/4	0.0140(3)	0.0144(3)	0.0350(4)	0	0	0
Sr(2)	4*c*	0	0.55585(3)	1/4	0.0127(2)	0.0128(3)	0.0118(2)	0	0	0
Si(1)	8*f*	0	0.05282(5)	0.5834(2)	0.0155(5)	0.0126(5)	0.0101(5)	0	0	0.0005(4)
Si(2)	4*c*	0	0.72110(8)	1/4	0.0120(7)	0.0134(7)	0.0117(7)	0	0	0
Mg/Li(1) [a]	8*f*	0	0.1906(1)	0.0529(3)	0.016(1)	0.017(1)	0.013(1)	0	0	–0.0017(9)

a: Mg/Li(1) = 0.502(8)Mg + 0.498Li

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