hedral holes. Despite the low scattering power of V for neutrons, neutron diffraction was used because N has a large scattering power. Hence, in this experiment the structure was determined solely by the N atom positions. The investigation confirmed that β-V_2N has the ε-Fe_2N structure, similar to β-Nb_2N and β-Ta_2N.

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Structure of Dilithium Zinc Silicate γ_{II}-Li_2ZnSiO_4

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Abstract. Li_2ZnSiO_4, monoclinic, $P2_1/n$, $a = 6{\cdot}262\ (3)$, $b = 10{\cdot}602\ (4)$, $c = 5{\cdot}021\ (4)$ Å, $\beta = 90{\cdot}51\ (5)°$, $Z = 4$, $D_x = 3{\cdot}41$ Mg m^{-3}, μ(Mo $K\alpha$) = 7·65 mm^{-1}. Crystals were twinned on (001) with a as the twin axis. The structure of the γ_{II} modification has been solved by the heavy-atom method and refined by the least-squares method to $R = 0{\cdot}060$ for 772 observed reflections with the twin ratio 0·65:0·35. All cations are coordinated tetrahedrally by O atoms.

Introduction. Setoguchi & Sakamoto (1974) and Setoguchi (1979) have synthesized the compounds $Li_2M^{2+}SiO_4$ (M = Zn, Mg) by a flux method. In this paper we deal with the structure determination of γ_{II}-Li_2ZnSiO_4 as part of a systematic study of these compounds.

Crystals of γ_{II}-Li_2ZnSiO_4 were grown from a Li_2MoO_4 solvent by a slow-cooling flux method. They were granular in shape with diameters ranging from 0·1 to 0·5 mm. Weissenberg photographs about **b** of all crystals examined showed a double-lattice character, indicating that the crystals were twinned on (001). Further visual intensity estimations of the double spots gave twin ratios approximately equal to 0·6:0·4 for all the crystals. The photographs also showed monoclinic symmetry with systematic absences $0k0$ for k odd and $h0l$ for $h + l$ odd, indicating the space group $P2_1/n$. A roughly spherical crystal of diameter 0·2 mm was selected for the data collection. Cell dimensions and intensity data were measured on a Rigaku four-circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation. The cell dimensions were determined by a least-squares fit to the setting angles of 25 reflections from the larger of the twin components. Intensities were collected using the ω–2θ scan technique with a scan range of $(1{\cdot}2 + 0{\cdot}5 \tan\theta)°$. By using a receiving slit with a large aperture (5·5 × 5·5 mm), the intensities of pairs of reflections, hkl and $h\bar{k}\bar{l}$, from the two twin components could be collected at the same time. The measured intensities of 1635 reflections ($2\theta < 55°$) were averaged to yield a set of 772 symmetrically independent values, $I_o(hkl)$, after Lp corrections. No correction was made for absorption.

The intensities $I(hkl)$ and $I(h\bar{k}\bar{l})$ were separated from the observed intensities $I_o(hkl)$ and $I_o(h\bar{k}\bar{l})$ according to the following equations (Nes & Vos, 1978):

$$I_o(hkl) = w_1\, I(hkl) + w_2\, I(h\bar{k}\bar{l})$$
$$I_o(h\bar{k}\bar{l}) = w_2\, I(hkl) + w_1\, I(h\bar{k}\bar{l}),$$

where hkl refer to the larger of the twin components, and w_1/w_2 ($w_1 + w_2 = 1$) is the twin ratio. The initial set of intensity data was obtained for $w_1 = 0{\cdot}6$.

A three-dimensional Patterson map revealed positions of the Zn atoms, and the Si and O atoms were located from subsequent Fourier maps. Refinements of

Table 1. *Final atomic coordinates with their e.s.d.'s*

	x	y	z
Zn	0·4986 (1)	0·1647 (1)	0·3095 (1)
Si	0·2474 (3)	0·4124 (2)	0·3135 (3)
Li(1)	−0·0088 (19)	0·1603 (12)	0·3033 (12)
Li(2)	0·2381 (21)	0·0765 (12)	0·7157 (25)
O(1)	0·2484 (8)	0·4092 (4)	0·6378 (9)
O(2)	0·2551 (7)	0·5564 (4)	0·2072 (9)
O(3)	0·0329 (7)	0·3414 (4)	0·2033 (9)
O(4)	0·4596 (7)	0·3387 (4)	0·2094 (9)

Table 2. *Selected bond distances* (Å) *and angles* (°)

				O–M–O angles
SiO$_4$ tetrahedron				
Si–O(1)	1·629 (5)	O(1)–O(2)	2·667 (7)	110·5 (3)
–O(2)	1·617 (5)	–O(3)	2·654 (7)	109·0 (3)
–O(3)	1·632 (5)	–O(4)	2·643 (7)	108·3 (3)
–O(4)	1·632 (5)	O(2)–O(3)	2·670 (6)	110·5 (3)
		–O(4)	2·639 (6)	108·6 (3)
		O(3)–O(4)	2·672 (6)	109·9 (2)
ZnO$_4$ tetrahedron				
Zn–O(1)	1·956 (5)	O(1)–O(2)	3·274 (7)	113·4 (2)
–O(2)	1·961 (5)	–O(3)	3·235 (7)	110·2 (2)
–O(3)	1·988 (5)	–O(4)	3·212 (7)	111·6 (2)
–O(4)	1·927 (5)	O(2)–O(3)	2·934 (6)	95·0 (2)
		–O(4)	3·310 (6)	116·7 (2)
		O(3)–O(4)	3·160 (6)	107·6 (2)
Li(1)O$_4$ tetrahedron				
Li(1)–O(1)	1·88 (1)	O(1)–O(2)	3·219 (7)	115·3 (7)
–O(2)	1·93 (1)	–O(3)	3·214 (7)	111·8 (6)
–O(3)	2·00 (1)	–O(4)	3·237 (7)	110·9 (6)
–O(4)	2·05 (1)	O(2)–O(3)	3·329 (6)	115·5 (6)
		–O(4)	2·979 (6)	96·7 (6)
		O(3)–O(4)	3·215 (6)	105·0 (6)
Li(2)O$_4$ tetrahedron				
Li(2)–O(1)	1·92 (2)	O(1)–O(2)	3·257 (7)	106·7 (6)
–O(2)	2·13 (2)	–O(3)	3·280 (7)	111·6 (6)
–O(3)	2·04 (2)	–O(4)	3·324 (7)	117·7 (7)
–O(4)	1·96 (2)	O(2)–O(3)	2·934 (6)	89·2 (6)
		–O(4)	2·979 (6)	93·2 (6)
		O(3)–O(4)	3·590 (6)	127·4 (7)

the atomic parameters for various values of w_1 (0·55–0·70) were carried out by the block-diagonal least-squares method (*HBLS* V; Ashida, 1973) with isotropic temperature factors and unit weights. The R value thus obtained was 0·103 for $w_1 = 0·64$. A subsequent difference map revealed positions of the remaining Li atoms. Further refinements with isotropic temperature factors for the Li atoms and anisotropic temperature factors for the Zn, Si and O atoms gave the final R of 0·060 for $w_1 = 0·65$. Atomic scattering factors for Zn^{2+}, Si, Li$^+$ and O$^-$ were taken from *International Tables for X-ray Crystallography* (1974). Final positional parameters are given in Table 1.* All computations were made on an ACOS System 800 computer of the Computation Center of Osaka University.

Discussion. Fig. 1 shows the structure viewed along **c**. The structure is based on a distorted hexagonal-close-packing arrangement of O atoms with layers stacked parallel to (001). All cations are coordinated tetrahedrally by O atoms. The ZnO$_4$ and Li(1)O$_4$ tetrahedral pairs share corners to form a chain along **a**, and these chains are held together through other corners, thus forming puckered layers parallel to (010). Similarly the SiO$_4$ and Li(2)O$_4$ tetrahedral pairs form a chain along **a**, and these chains also form puckered layers parallel to (010). These two kinds of layers are held together through common corners or edges to form a three-dimensional framework. The same type of framework is seen in the high-temperature form of Li$_3$PO$_4$ (Zemann, 1960) and in Zn–Li silicate (Yu, Smith & Austerman, 1978).

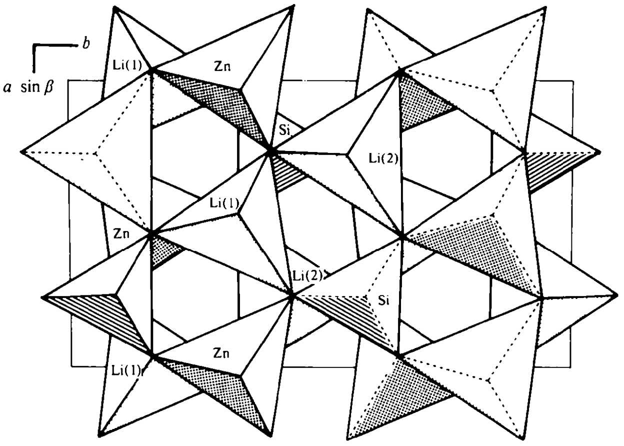

Fig. 1. The crystal structure viewed along **c**.

Selected bond distances and angles are listed in Table 2. The SiO$_4$ tetrahedra are quite regular with a mean Si–O distance of 1·628 Å. On the other hand the ZnO$_4$ tetrahedra are significantly distorted. The Zn–O distances range from 1·927 (5) to 1·988 (5) Å with a mean value of 1·958 Å which is normal for a coordination tetrahedron about Zn. The LiO$_4$ tetrahedra also show marked departures from a regular tetrahedron. The Li–O distances range from 1·88 (1) to 2·05 (1) Å for Li(1) and from 1·92 (2) to 2·13 (2) Å for Li(2) with mean values of 1·97 and 2·01 Å respectively. These mean values may be compared with the values of 1·96 and 1·99 Å in Li$_3$PO$_4$ and 1·959 and 2·009 Å in Li$_2$BeSiO$_4$ (Howie & West, 1974) for the corresponding Li(1) and Li(2) tetrahedral sites. It is to be noted that the coordination tetrahedra at the Li(2)

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* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34640 (5 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

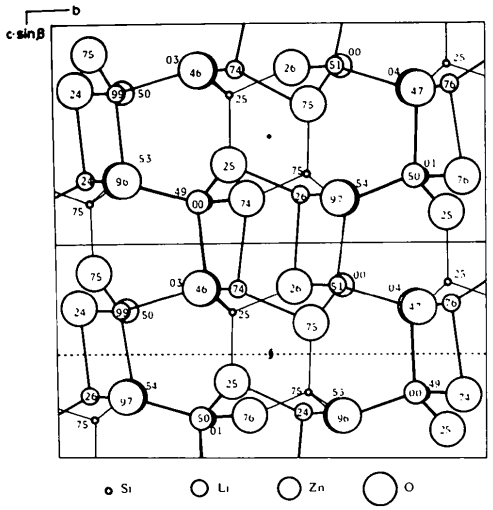

Fig. 2. Relative orientations of the twin components at the twin boundary. The twin boundary is shown by the broken line. The fractional *a* coordinates are shown as percentages of the *a* length.

sites in the above compounds are all more distorted than those at the Li(1) sites.

Fig. 2 shows a probable model for twinning. The twin symmetry relating the two twin components is 2_1 parallel to **a**, by which the arrangements of the O, Si and Li(2) atoms remain almost unchanged since originally they have pseudo 2_1 symmetry. The positions of the Zn and Li(1) atoms are also approximately related to each other by 2_1 symmetry, and further Zn^{2+} and Li^+ ions in fourfold coordination have nearly equal effective ionic radii (Whittaker & Muntus, 1970). Therefore the ZnO_4 and $Li(1)O_4$ tetrahedra at the twin boundary do not suffer significant distortions.

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Structure of Cobalt Dilithium Silicate β_{II}-Li_2CoSiO_4

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Abstract. Li_2CoSiO_4, orthorhombic, $Pbn2_1$, $a = 6{\cdot}253$ (5), $b = 10{\cdot}685$ (9), $c = 4{\cdot}929$ (9) Å, $Z = 4$, $D_x = 3{\cdot}33$ Mg m^{-3}, μ(Mo $K\alpha$) = 5·50 mm^{-1}. The structure of the β_{II} modification has been solved by the heavy-atom method and refined by the least-squares method to $R = 0{\cdot}044$ for 789 observed reflections. The Co^{2+} ion is coordinated tetrahedrally by O atoms. The Co—O distances range from 1·966 (5) to 1·983 (6) Å with a mean of 1·975 Å.

Introduction. Crystals of β_{II}-Li_2CoSiO_4 were grown from a LiCl flux (Setoguchi, 1979). They were granular in shape with diameters ranging from 0·3 to 2 mm. Weissenberg photographs of all 17 crystals examined

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