

Colorless crystals of the title compounds were of commercial-grade material (Merck). They are hygroscopic and were held in a capillary. Oscillation and Weissenberg photographs, as well as preliminary diffractometer data collection suggested the isomorphism of the crystals. The structure of  $K_5Na(HPO_4)_3$  was solved by direct methods and a satisfactory solution was obtained in the non-centrosymmetric space group  $Pna2_1$ . The refinement for  $K_2HPO_4$  was started by using the coordinates for the heavy atoms of  $K_5Na(HPO_4)_3$ . In both structures the H atoms were found from difference maps and refined with constraints ( $O-H = 0.97 \text{ \AA}$ ). *SHELX76* (Sheldrick, 1976) was used for the refinements.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71731 (42 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: DU1064]

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## LiGaSi<sub>2</sub>O<sub>6</sub>

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## Abstract

The structure of gallium lithium metasilicate,  $LiGaSi_2O_6$ , has been determined from diffractometer data. The structure is similar to that of spodumene ( $LiAlSi_2O_6$ ).

## Comment

The structure of the title compound is isostructural with  $LiAlSi_2O_6$  and  $LiFeSi_2O_6$  (Clark, Appleman & Papike, 1969),  $LiScSi_2O_6$  (Hawthorne & Grundy, 1977) and  $LiInSi_2O_6$  (Grotepass, Behruzi & Hahn, 1983). This structure ( $C2/c$ ) takes the high-temperature form of  $LiFeSi_2O_6$  and  $LiCrSi_2O_6$ , which transform to the low-temperature form ( $P2_1/c$ )

at 228 and 343 K, respectively (Behruzi, Hahn, Pre-witt & Baldwin, 1984).

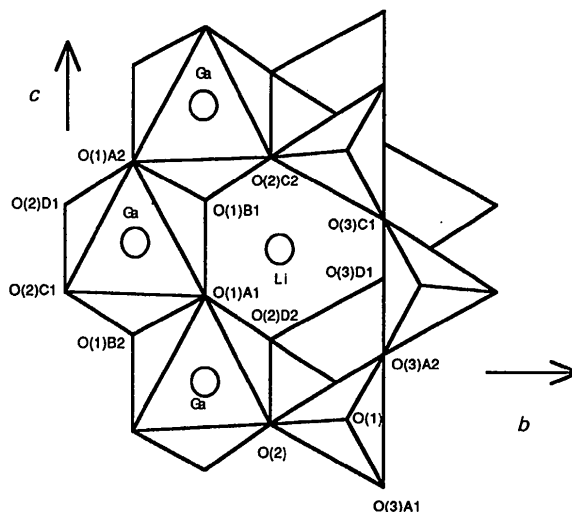


Fig. 1.  $a^*$ -axis projection of  $LiGaSi_2O_6$ . Atom nomenclature follows that used by Clark, Appleman & Papike (1969).

## Experimental

The title compound was prepared according to the procedure described by Ohashi, Osawa & Sato (1989).

### Crystal data

$LiGaSi_2O_6$

$M_r = 228.83$

Monoclinic

$C2/c$

$a = 9.561 (1) \text{ \AA}$

$b = 8.569 (1) \text{ \AA}$

$c = 5.268 (1) \text{ \AA}$

$\beta = 110.244 (3)^\circ$

$V = 404.90 (5) \text{ \AA}^3$

$Z = 4$

$D_x = 3.75 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 22 reflections

$\theta = 33-37^\circ$

$\mu = 7.29 \text{ mm}^{-1}$

$T = 298 \text{ K}$

$0.20 \times 0.15 \times 0.11 \text{ mm}$

Colourless

### Data collection

Enraf-Nonius CAD-4

diffractometer

$\omega$ -2 $\theta$  scans

Absorption correction:

by integration from crystal shape

$T_{\min} = 0.371$ ,  $T_{\max} = 0.501$

1309 measured reflections

1309 independent reflections

1268 observed reflections

$[I > 1.5\sigma(I)]$

$\theta_{\max} = 40^\circ$

$h = 0 \rightarrow 17$

$k = 0 \rightarrow 15$

$l = -9 \rightarrow 9$

3 standard reflections

monitored every 100

reflections for orientation and every 240 min for intensity

intensity variation:  $-0.8\%$

### Refinement

Refinement on  $F$

$R = 0.017$

Extinction correction:

isotropic secondary

$wR = 0.038$   
 $S = 1.7$   
 1268 reflections  
 48 parameters  
 $w = 1/\sigma^2(F)$   
 $(\Delta/\sigma)_{\max} < 0.005$   
 $\Delta\rho_{\max} = 0.6 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -1.0 \text{ e } \text{\AA}^{-3}$

Extinction coefficient:  
 $12.6 \times 10^{-6}$   
 Atomic scattering factors,  
 including  $f'$  and  $f''$ , from  
*International Tables for*  
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Clark, J. R., Appleman, D. E. & Papike, J. J. (1969). *Mineral. Soc. Am. Spec. Pap.* **2**, 31–50.  
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Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	$U_{\text{eq}}$
Li	0	0.2642 (5)	1/4	0.0184 (7)
Ga	0	0.90154 (2)	1/4	0.00461 (3)
Si	0.29673 (3)	0.09112 (3)	0.26088 (6)	0.00443 (5)
O(1)	0.11357 (8)	0.08377 (8)	0.1442 (1)	0.0054 (1)
O(2)	0.36547 (8)	0.26160 (9)	0.3232 (1)	0.0086 (1)
O(3)	0.35682 (7)	0.0001 (1)	0.0491 (2)	0.0096 (1)

Table 2. Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Si tetrahedron		Ga octahedron	
Si—O(1)	1.644 (1)	Ga—O(1)A1,B1	2.085 (1)
Si—O(2)	1.589 (1)	Ga—O(1)A2,B2	1.987 (1)
Si—O(3)A1	1.620 (1)	Ga—O(2)C1,D1	1.893 (1)
Si—O(3)A2	1.626 (1)	Mean of six	1.988
Mean of four	1.620		
O(1)—O(2)	2.728 (1)	O(1)A1—O(1)B1	2.763 (1)
O(1)—O(3)A1	2.642 (1)	O(2)C1—O(2)D1	2.930 (1)
O(1)—O(3)A2	2.654 (1)	O(1)A1—O(2)C1 × 2	2.769 (1)
O(2)—O(3)A1	2.651 (1)	O(1)A1—O(1)A2 × 2	3.000 (1)
O(2)—O(3)A2	2.554 (1)	O(1)A2—O(2)C1 × 2	2.863 (1)
O(3)A1—O(3)A2	2.634 (1)	O(1)A2—O(2)D1 × 2	2.732 (1)
Si—Si	3.0620 (4)	O(1)A1—O(1)B2 × 2	2.608 (1)
		Ga—Ga	3.1280 (1)
O(1)—Si—O(2)	115.05 (4)	O(1)A1—Ga—O(1)B1	83.00 (3)
O(1)—Si—O(3)A1	108.04 (4)	O(1)A1—Ga—O(2)C1 × 2	88.08 (3)
O(1)—Si—O(3)A2	108.49 (4)	O(1)A1—Ga—O(1)A2 × 2	94.88 (3)
O(2)—Si—O(3)A1	111.39 (5)	O(1)A1—Ga—O(1)B2 × 2	79.63 (3)
O(2)—Si—O(3)A2	105.19 (4)	O(1)A2—Ga—O(2)C1 × 2	95.10 (3)
O(3)A1—Si—O(3)A2	108.46 (4)	O(1)A2—Ga—O(2)D1 × 2	89.51 (3)
		O(2)C1—Ga—O(2)D1	101.40 (3)
Li antiprism		Si—O(3)—Si	141.21 (5)
Li—O(1)A1,B1	2.073 (3)	Ga—O(1)—Ga	100.37 (3)
Li—O(2)C2,D2	2.181 (1)	O(3)—O(3)—O(3)	180.00 (1)
Li—O(3)C1,D1	2.466 (3)		
Mean of six	2.240		

The calculations were initiated with the atomic parameters of LiAlSi<sub>2</sub>O<sub>6</sub> given by Clark, Appleman & Papike (1969). All calculations were performed with the SDP program system (B. A. Frenz & Associates, Inc., 1982).

Lists of structure factors and anisotropic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71629 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: OH1040]

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## Strontium Cobalt(II) Diarsenate

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## Abstract

The novel compound, SrCoAs<sub>2</sub>O<sub>7</sub>, has been obtained from a hydrothermal reaction. SrCoAs<sub>2</sub>O<sub>7</sub> adopts a tunnel structure and its framework consists of corner-sharing CoO<sub>5</sub> square pyramids and As<sub>2</sub>O<sub>7</sub> groups. Sr atoms are located in the pentagonal-shaped tunnels, which are formed by the edges of two square pyramids and three arsenate tetrahedra.

## Comment

Recently, a large number of new structures in the A–V–P–O system, where A includes alkali, alkaline-earth and transition-metal cations, have been synthesized under hydrothermal conditions (Kang, Lee, Wang & Lii, 1992; Lii, 1992; Lii, Wen, Su & Chueh, 1992). These phosphates show a variety of new structural types with tunnel or layer structures. However, little structural work on transition-metal arsenates has been reported. Recently, we noted that single crystals of VO(H<sub>2</sub>AsO<sub>4</sub>)<sub>2</sub> could be grown under hydrothermal conditions (Wang & Lee, 1991). Subsequent research revealed that many vanadium arsenates containing alkali or alkaline-earth metals can also be obtained by hydrothermal methods (Cheng & Wang, 1992; Wang & Cheng, 1993). The present study is an extension of our previous work on the cobalt arsenate system.

The title compound was obtained as violet crystals by heating a reaction mixture of Co(OH)<sub>2</sub> (0.4639 g), Sr(OH)<sub>2</sub>·8H<sub>2</sub>O (1.3267 g) and 12 ml 13.3% aq. H<sub>3</sub>AsO<sub>4</sub> in a 23 ml teflon-lined autoclave at 503 K for 4 d followed by slow cooling (5 K h<sup>-1</sup>) to room temperature.