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*Acta Cryst.* (1995). C51, 1972–1975

## Caesium–Lithium Phyllosilicate, Cs<sub>1.33</sub>Li<sub>0.67</sub>Si<sub>2</sub>O<sub>5</sub>

NORA VELDMAN AND ANTHONY L. SPEK

*Bijvoet Center for Biomolecular Research,  
 Department of Crystal and Structural Chemistry,  
 Utrecht University, Padualaan 8, 3584 CH Utrecht,  
 The Netherlands*

HENDRIKA T. J. SUPÈR AND BERNARD H. W. S. DE JONG

*Institute for Earth Sciences and Vening Meinesz  
 Institute for Geodynamic Research, Utrecht University,  
 PO Box 80021, 3508 TA Utrecht, The Netherlands*

(Received 8 February 1995; accepted 18 April 1995)

### Abstract

The crystal structure of a (Cs,Li) phyllosilicate with composition Cs<sub>1.33</sub>Li<sub>0.67</sub>Si<sub>2</sub>O<sub>5</sub> has been characterized by a single-crystal X-ray diffraction study. Its silica sheet is exceedingly tortuous with a four-eight-twelve-membered ring topology and a large variation in bridging-oxygen number density in the sheet, thus differing from the six-membered ring topology of Li phyllosilicate and the four-eight-membered ring topology in Cs and Rb phyllosilicate. The title compound lacks the characteristic sandwich structure of sheet silicates. It resembles a three-dimensional network in which Si atoms are replaced by strictly threefold O-coordinated Li atoms which form flat sheets at  $ca\ y = 0$  and  $y = \frac{1}{2}$  with seven- to twelvefold O-coordinated Cs atoms between the silica–lithium sheets at  $y = \frac{1}{4}$  and  $y = \frac{3}{4}$ . The Cs atoms recur in two types of honeycomb tunnels parallel to the  $b$  axis.

### Comment

As part of a study on alkali phyllosilicates and the effect of sheet tortuosity on <sup>29</sup>Si MASNMR chemical shifts, we have prepared transparent colourless (Cs,Li) phyllosilicate crystals from a Li<sub>2</sub>O.Cs<sub>2</sub>O.4SiO<sub>2</sub> glass. The chemical composition of the crystals is Cs<sub>1.33</sub>Li<sub>0.67</sub>Si<sub>2</sub>O<sub>5</sub>, indicating incongruent precipitation. The crystals are not markedly hygroscopic and none of the special measures needed to prevent Cs phyllosilicate from decomposing is required.

The title compound exhibits a new structure type with extreme tortuosity of the silica sheet (Fig. 1). The individual chains (*i.e.* –Si6'–Si1–Si2–Si3–Si4–Si5–Si6–Si1''–) which make up the sheets are 'sechser chains' according to the Liebau (1985) classification, the overall classification of the silica sheet being an unbranched *sechser* single layer. Each Si atom is bonded with two bridging O atoms, O(*br*), in the chain direction and with one O(*br*) perpendicular to that direction, connecting the individual chains into a sheet. The interchain O(*br*)

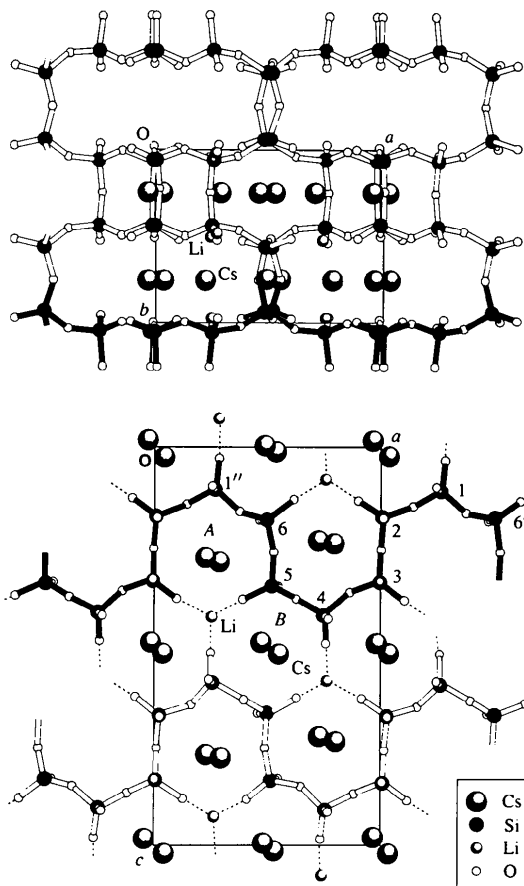


Fig. 1. Projections of the sheet structure of Cs<sub>1.33</sub>Li<sub>0.67</sub>Si<sub>2</sub>O<sub>5</sub>. The *sechser* chain is indicated in black. Top: silica sheet. A similar sheet, generated by the twofold screw axis along  $b$ , completes the unit-cell contents. Bottom: the chicken-wire Li–silicate sheet.

atoms on Si5 and Si6 link adjacent chains, resulting in a four-membered ring. The other four interchain O(*br*) atoms are rotated to the opposite side, resulting in four interchain bonds in that direction. As a result, each chain is involved on one side in a sequence of three four-membered rings and one eight-membered ring and on the other side in a sequence of one four-membered and one twelve-membered ring. Thus, the number density of Si—O(*br*) linkages in the sheet shows large variations in opposite directions.

The non-bridging O atoms, O(*nbr*), are bonded to Li atoms, which connect the silica sheets. These O(*nbr*) atoms point either to the sheet above or, for the other half, to the sheet below. Each Li atom is thus involved in planar threefold coordination by O(*nbr*) atoms. The Li atoms are located in the *ac* plane at approximately  $y = 0$  and  $y = \frac{1}{2}$ , and, together with the silica chains, form a chicken-wire network consisting of six-membered rings perpendicular to the silica sheets. Two types of honeycomb-shaped tunnels are produced, bounded by either five Si tetrahedra and one Li atom or by four Si tetrahedra and two Li atoms, denoted in Fig. 1 by *A* and *B*, respectively. The Cs atoms are trapped in pockets in the tunnels. The 'curtain' character of the Li-silica sheets offers a possible reason for the observation that (Cs,Li) phyllosilicate is not hygroscopic at all in spite of its high Cs content, in contrast to the exceedingly hygroscopic Cs phyllosilicate (de Jong, Slaats, Supèr, Veldman & Spek, 1994).

The Cs ions filling the honeycombs are located on the crystallographic mirror planes at  $y = \frac{1}{4}$  and  $y = \frac{3}{4}$ . Two types of Cs atoms exist. One type fills the type-*B* tunnels, forming a zone of Cs atoms resembling the alkali layer in standard phyllosilicate. The other fills type-*A* tunnels. All Cs atoms function as channel fillers rather than as structural pillars. Their O-atom coordination is irregular (ranging from 7 to 12) and no simple polyhedral coordination sphere can be assigned.

In summary, (Cs,Li) phyllosilicate is a curiosity among sheet silicates. The standard sheet silicate sandwich characteristic with a clear-cut separation between silica sheet and alkali zones is not well defined here. However, we can stretch the concept and describe the structure as an alternation of Cs and Li-silica zones perpendicular to the *b* axis that are strictly separated from one another. The strictly threefold O-coordinated Li atom, with O—Li—O angles summing to 359°, is the first one we have encountered. Li atoms with close to threefold coordination are found, for instance, in Li<sub>4</sub>SiO<sub>4</sub> (de Jong, Ellerbroek & Spek, 1994) and Li<sub>3</sub>Zn<sub>0.5</sub>GeO<sub>4</sub> (Plattner & Völlenkne, 1979).

The Si atom is tetrahedrally coordinated by O atoms;  $\langle d[\text{Si—O}(\textit{nbr})] \rangle$  is 1.562 (4) Å [O(*nbr*) = O2, O6, O9, O12, O15, O18], which is in all instances shorter than  $\langle d[\text{Si—O}(\textit{br})] \rangle$  of 1.633 (5) Å. The O—Si—O angle varies between 103.0 (3) and 115.2 (2)°, and  $\langle \text{Si—O—Si} \rangle$  is 150.4 (3)°, with a variation between 137.2 (3)

and 174.8 (5)°. Interestingly, the average O(*nbr*)—Si—O(*br*) angle of 113.2° [range 110.4 (3)—115.4 (2)°] is significantly larger than the average O(*br*)—Si—O(*br*) angle of 105.5° [range 103.1 (2)—107.1 (3)°].

The (Cs,Li) phyllosilicate structure exhibits pseudo *A*-centring, indicated by the *MISSYM* (Le Page, 1987) algorithm as implemented in *PLATON* (Spek, 1990). This *A*-centred lattice symmetry is broken by the fact that Si tetrahedra that should have the same orientation take different orientations, mainly affecting the O-atom positions. Interestingly, preliminary work on the structure of the isostructural (Rb,Li) phyllosilicate shows that that compound crystallizes with exact *A*-centring with both silicon tetrahedra orientations present at the same site, but as disorder forms.

Valence-strength calculations for the atoms in this structure were performed using the parametrization of Brese & O'Keeffe (1991). For the six Si atoms the average valence sum is  $-4.12$  [range  $-4.07$  to  $-4.16$ ], for the two Li atoms it is  $-1.09$ , for the eight Cs atoms  $-0.95$  [range  $-0.88$  to  $-1.07$ ] and for the eighteen O atoms  $2.06$  [range  $1.85$  to  $2.22$ ] (de Jong, Slaats, Supèr, Veldman & Spek, 1994).

## Experimental

(Cs,Li) phyllosilicate crystals were prepared from a Li<sub>2</sub>O—Cs<sub>2</sub>O·4SiO<sub>2</sub> glass. This glass was heated at the rate of 10 K min<sup>-1</sup> to 1288 K, kept at that temperature for 0.5 h, and cooled at a rate of 0.06 K min<sup>-1</sup> to 1118 K, followed by a quench to room temperature. X-ray data were collected for a thin and irregular plate-shaped crystal selected from the crucible-crystallized glass. The crystal was cut to size to fit in the homogeneous part of the X-ray beam and glued on top of a Lindemann glass capillary. Reflection profiles showed the large anisotropic mosaicity expected for this type of sheet structure.

### Crystal data

Cs<sub>1.33</sub>Li<sub>0.67</sub>Si<sub>2</sub>O<sub>5</sub>  
 $M_r = 318.00$   
 Monoclinic  
 $P2_1/m$   
 $a = 10.9547$  (9) Å  
 $b = 8.4281$  (7) Å  
 $c = 18.962$  (2) Å  
 $\beta = 90.314$  (7)°  
 $V = 1750.7$  (3) Å<sup>3</sup>  
 $Z = 12$   
 $D_x = 3.619$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
 $\lambda = 0.71073$  Å  
 Cell parameters from 25 reflections  
 $\theta = 11.4$ – $14.0$ °  
 $\mu = 8.74$  mm<sup>-1</sup>  
 $T = 150$  K  
 Thin plate  
 $0.50 \times 0.40 \times 0.05$  mm  
 Colourless

### Data collection

Enraf-Nonius CAD-4T  
 rotating-anode diffractometer  
 $\omega/2\theta$  scans

3692 observed reflections  
 $[I > 2\sigma(I)]$   
 $R_{\text{int}} = 0.09$   
 $\theta_{\text{max}} = 27.45$ °

Absorption correction:  $h = -13 \rightarrow 14$   
 analytical  $k = 0 \rightarrow 10$   
 $T_{\min} = 0.070$ ,  $T_{\max} = 0.691$   
 $l = -24 \rightarrow 24$   
 3 standard reflections  
 8537 measured reflections frequency: 60 min  
 4261 independent reflections intensity decay: 2%

## Refinement

Refinement on  $F^2$   
 $R(F) = 0.0394$   
 $wR(F^2) = 0.144$   
 $S = 1.13$   
 4258 reflections  
 266 parameters  
 $w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 2.969P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = -0.004$   
 $\Delta\rho_{\max} = 2.997 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -2.308 \text{ e } \text{Å}^{-3}$

Extinction correction:  
 SHELXL93 (Sheldrick,  
 1993)  
 Extinction coefficient:  
 0.0020 (1)  
 Atomic scattering factors  
 from *International Tables*  
 for *Crystallography* (1992,  
 Vol. C, Tables 4.2.6.8 and  
 6.1.1.4)

Si3—O7	1.643 (4)	Cs3···O9	3.498 (4)
Si3—O8	1.6232 (17)	Cs4···O9 <sup>iv</sup>	3.165 (4)
Si3—O9	1.562 (4)	Cs4···O9 <sup>vii</sup>	3.165 (4)
Si3—O10	1.647 (4)	Cs4···O7 <sup>iv</sup>	3.169 (4)
Si4—O10	1.632 (4)	Cs4···O7 <sup>vii</sup>	3.169 (4)
Si4—O11	1.6245 (19)	Cs4···O17 <sup>iv</sup>	3.232 (6)
Si4—O12	1.562 (4)	Cs4···O15 <sup>iii</sup>	3.266 (4)
Si4—O13	1.631 (4)	Cs4···O15 <sup>vi</sup>	3.266 (4)
Si5—O13	1.625 (4)	Cs4···O4 <sup>iv</sup>	3.331 (4)
Si5—O14	1.640 (2)	Cs4···O4 <sup>vii</sup>	3.331 (4)
Si5—O15	1.564 (4)	Cs5···O12 <sup>ix</sup>	3.033 (4)
Si5—O16 <sup>i</sup>	1.630 (4)	Cs5···O12 <sup>x</sup>	3.033 (4)
Si6—O1	1.632 (4)	Cs5···O13 <sup>viii</sup>	3.022 (4)
Si6—O16	1.644 (4)	Cs5···O13 <sup>xi</sup>	3.272 (4)
Si6—O17	1.636 (2)	Cs5···O14 <sup>xv</sup>	3.275 (6)
Si6—O18	1.553 (4)	Cs5···O15 <sup>viii</sup>	3.365 (4)
Li1—O6 <sup>ii</sup>	1.830 (10)	Cs5···O15 <sup>xi</sup>	3.365 (4)
Li1—O2 <sup>iii</sup>	1.843 (10)	Cs6···O12 <sup>ix</sup>	3.022 (4)
Li1—O18 <sup>iv</sup>	1.847 (10)	Cs6···O12 <sup>x</sup>	3.022 (4)
Li2—O15 <sup>ii</sup>	1.815 (10)	Cs6···O9 <sup>x</sup>	3.187 (4)
Li2—O9 <sup>iv</sup>	1.832 (10)	Cs6···O9 <sup>xv</sup>	3.187 (4)
Li2—O12 <sup>v</sup>	1.870 (12)	Cs6···O11	3.427 (6)
Cs1···O6 <sup>vi</sup>	3.146 (4)	Cs6···O10 <sup>x</sup>	3.496 (4)
Cs1···O6 <sup>vi</sup>	3.146 (4)	Cs6···O10 <sup>ix</sup>	3.496 (4)
Cs1···O7 <sup>ii</sup>	3.153 (4)	Cs6···O9	3.536 (4)
Cs1···O7 <sup>ii</sup>	3.153 (4)	Cs6···O9 <sup>iv</sup>	3.536 (4)
Cs1···O7 <sup>vi</sup>	3.153 (4)	Cs7···O2 <sup>x</sup>	3.060 (4)
Cs1···O10 <sup>vi</sup>	3.287 (4)	Cs7···O2 <sup>iii</sup>	3.060 (4)
Cs1···O10 <sup>ii</sup>	3.287 (4)	Cs7···O18 <sup>iv</sup>	3.233 (4)
Cs1···O14 <sup>vi</sup>	3.288 (6)	Cs7···O18	3.233 (4)
Cs1···O18 <sup>iv</sup>	3.432 (4)	Cs7···O18 <sup>x</sup>	3.375 (5)
Cs1···O18 <sup>viii</sup>	3.432 (4)	Cs7···O18 <sup>viii</sup>	3.375 (5)
Cs1···O16 <sup>vi</sup>	3.491 (4)	Cs7···O17 <sup>viii</sup>	3.384 (6)
Cs1···O16 <sup>vii</sup>	3.491 (4)	Cs2···O3	3.461 (6)
Cs2···O16	3.120 (4)	Cs8···O2 <sup>iv</sup>	3.162 (4)
Cs2···O16 <sup>iv</sup>	3.120 (4)	Cs8···O2 <sup>vii</sup>	3.162 (4)
Cs2···O18 <sup>iv</sup>	3.235 (5)	Cs8···O4 <sup>iv</sup>	3.217 (4)
Cs2···O18	3.235 (5)	Cs8···O4 <sup>vii</sup>	3.217 (4)
Cs2···O5 <sup>viii</sup>	3.388 (7)	Cs8···O6 <sup>iv</sup>	3.317 (4)
Cs2···O13 <sup>viii</sup>	3.473 (4)	Cs8···O6 <sup>vii</sup>	3.317 (4)
Cs2···O13 <sup>iii</sup>	3.473 (4)	Cs8···O6 <sup>xi</sup>	3.496 (4)
Cs2···O6 <sup>viii</sup>	3.513 (4)	Cs8···O6 <sup>xii</sup>	3.496 (4)
Cs2···O6 <sup>ii</sup>	3.513 (4)	Cs8···O5 <sup>xiii</sup>	3.556 (6)
Cs2···O8 <sup>viii</sup>	3.523 (6)	Cs8···O3 <sup>xiii</sup>	3.582 (6)
Cs2···O10 <sup>viii</sup>	3.566 (4)		
Cs2···O10 <sup>ii</sup>	3.566 (4)		

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ( $\text{Å}^2$ )

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{eq}}$
Si1	0.24914 (12)	0.0591 (2)	0.09546 (8)	0.0041 (3)
Si2	-0.00473 (13)	0.0580 (2)	0.16529 (8)	0.0041 (4)
Si3	-0.01724 (12)	0.0577 (2)	0.32905 (8)	0.0045 (4)
Si4	-0.25540 (12)	0.0598 (2)	0.41217 (8)	0.0035 (3)
Si5	-0.49489 (12)	-0.0637 (2)	0.33536 (8)	0.0046 (4)
Si6	0.48539 (13)	-0.0620 (2)	0.16995 (8)	0.0049 (4)
O1	0.3587 (3)	0.0332 (5)	0.1533 (2)	0.0117 (12)
O2	0.2701 (3)	-0.0253 (5)	0.0230 (2)	0.0110 (12)
O3	0.2339 (5)	1/4	0.0878 (3)	0.0090 (16)
O4	0.1270 (3)	-0.0029 (5)	0.1362 (2)	0.0097 (12)
O5	0.0016 (5)	1/4	0.1692 (3)	0.0110 (16)
O6	-0.1153 (3)	-0.0064 (5)	0.1209 (2)	0.0124 (12)
O7	-0.0103 (3)	-0.0043 (5)	0.2470 (2)	0.0083 (12)
O8	-0.0189 (5)	1/4	0.3244 (3)	0.0100 (17)
O9	0.0905 (3)	-0.0091 (5)	0.3744 (2)	0.0133 (12)
O10	-0.1537 (3)	0.0015 (5)	0.3552 (2)	0.0096 (11)
O11	-0.2375 (5)	1/4	0.4215 (3)	0.0093 (16)
O12	-0.2466 (3)	-0.0288 (5)	0.4844 (2)	0.0113 (12)
O13	-0.3868 (3)	0.0395 (5)	0.3723 (2)	0.0100 (12)
O14	-0.4530 (5)	-1/4	0.3413 (3)	0.0107 (17)
O15	-0.6233 (3)	-0.0271 (6)	0.3671 (2)	0.0133 (12)
O16	0.5156 (3)	-0.0151 (5)	0.2524 (2)	0.0093 (12)
O17	0.4484 (5)	-1/4	0.1689 (3)	0.0127 (17)
O18	0.5948 (3)	-0.0185 (6)	0.1219 (2)	0.0130 (12)
Cs1	0.77477 (4)	3/4	0.22906 (3)	0.0087 (1)
Cs2	0.70839 (4)	1/4	0.22505 (3)	0.0101 (2)
Cs3	0.27508 (4)	1/4	0.27806 (3)	0.0095 (2)
Cs4	0.20647 (4)	3/4	0.26565 (3)	0.0084 (1)
Cs5	0.45863 (4)	1/4	0.48606 (3)	0.0104 (2)
Cs6	0.02950 (4)	1/4	0.51657 (3)	0.0099 (2)
Cs7	0.51763 (4)	1/4	0.00835 (3)	0.0089 (2)
Cs8	0.03918 (4)	3/4	0.01696 (3)	0.0100 (2)
Li1	0.7397 (8)	0.5125 (13)	0.0726 (5)	0.010 (3)
Li2	0.2386 (8)	0.5203 (13)	0.4195 (6)	0.013 (3)

Table 2. Selected geometric parameters ( $\text{Å}$ , °)

Si1—O1	1.636 (4)	Cs3···O15 <sup>viii</sup>	3.086 (5)
Si1—O2	1.565 (4)	Cs3···O15 <sup>ii</sup>	3.086 (5)
Si1—O3	1.6240 (18)	Cs3···O1	3.130 (4)
Si1—O4	1.634 (4)	Cs3···O1 <sup>iv</sup>	3.130 (4)
Si2—O4	1.631 (4)	Cs3···O8	3.343 (6)
Si2—O5	1.6214 (17)	Cs3···O16	3.491 (4)
Si2—O6	1.568 (4)	Cs3···O16 <sup>iv</sup>	3.491 (4)
Si2—O7	1.637 (4)	Cs3···O9 <sup>iv</sup>	3.498 (4)

O6 <sup>ii</sup> —Li1—O2 <sup>iii</sup>	122.2 (5)	O11—Si4—O12	111.7 (3)
O6 <sup>ii</sup> —Li1—O18 <sup>iv</sup>	119.6 (5)	O11—Si4—O13	105.0 (3)
O2 <sup>iii</sup> —Li1—O18 <sup>iv</sup>	117.2 (5)	O12—Si4—O13	114.0 (2)
O15 <sup>ii</sup> —Li2—O9 <sup>iv</sup>	119.0 (6)	O13—Si5—O14	106.3 (2)
O15 <sup>ii</sup> —Li2—O12 <sup>v</sup>	120.4 (5)	O13—Si5—O15	112.5 (2)
O9 <sup>iv</sup> —Li2—O12 <sup>v</sup>	118.7 (5)	O13—Si5—O16 <sup>i</sup>	103.1 (2)
O1—Si1—O2	114.7 (2)	O14—Si5—O15	114.5 (3)
O1—Si1—O3	105.5 (3)	O14—Si5—O16 <sup>i</sup>	106.6 (3)
O1—Si1—O4	103.9 (2)	O15—Si5—O16 <sup>i</sup>	113.0 (2)
O2—Si1—O3	112.8 (3)	O1—Si6—O16	103.4 (2)
O2—Si1—O4	113.2 (2)	O1—Si6—O17	105.3 (2)
O3—Si1—O4	106.0 (3)	O1—Si6—O18	115.4 (2)
O4—Si2—O5	107.0 (3)	O16—Si6—O17	107.0 (3)
O4—Si2—O6	113.1 (2)	O16—Si6—O18	110.4 (2)
O4—Si2—O7	104.9 (2)	O17—Si6—O18	114.4 (3)
O5—Si2—O6	113.7 (3)	Si1—O1—Si6	144.6 (3)
O5—Si2—O7	106.2 (3)	Si1—O3—Si1 <sup>iv</sup>	164.4 (4)
O6—Si2—O7	111.4 (2)	Si1—O4—Si2	142.0 (3)
O7—Si3—O8	105.5 (3)	Si2—O5—Si2 <sup>iv</sup>	172.8 (4)
O7—Si3—O9	111.6 (2)	Si2—O7—Si3	142.8 (3)
O7—Si3—O10	103.9 (2)	Si3—O8—Si3 <sup>iv</sup>	173.6 (4)
O8—Si3—O9	113.5 (3)	Si3—O10—Si4	137.5 (3)
O8—Si3—O10	107.1 (3)	Si4—O11—Si4 <sup>iv</sup>	161.3 (4)
O9—Si3—O10	114.5 (2)	Si4—O13—Si5	153.5 (3)
O10—Si4—O11	106.7 (3)	Si5—O14—Si5 <sup>xiii</sup>	146.5 (4)
O10—Si4—O12	113.4 (2)	Si5 <sup>viii</sup> —O16—Si6	147.4 (3)
O10—Si4—O13	105.4 (2)	Si6—O17—Si6 <sup>xiii</sup>	151.3 (4)

Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $1 + x, \frac{1}{2} - y, z$ ; (iii)  $1 - x, \frac{1}{2} + y, -z$ ; (iv)  $x, \frac{1}{2} - y, z$ ; (v)  $-x, \frac{1}{2} + y, 1 - z$ ; (vi)  $1 + x, 1 + y, z$ ; (vii)  $x, 1 + y, z$ ; (viii)  $1 + x, y, z$ ; (ix)  $-x, -y, 1 - z$ ; (x)  $1 - x, -y, -z$ ; (xi)  $-x, 1 - y, -z$ ; (xii)  $-x, \frac{1}{2} + y, -z$ ; (xiii)  $x, -\frac{1}{2} - y, z$ .

Systematic absences are consistent with space groups  $P2_1$  and  $P2_1/m$ . The latter was adopted leading to a satisfactory refinement. No higher lattice symmetry was found with *LEPAGE* (Spek, 1988). General reflections with  $k + l = 2n + 1$  are systematically weaker but not extinct [the largest exceptions have an observed intensity of  $100\sigma(I)$ ], corresponding to pseudo *A*-centring of the structure. Inspection of the refined structure reveals that the major deviation from *A*-centring is caused by the position of the O atoms. An analytical method (Alcock, 1970) for absorption correction was applied as implemented in *PLATON* (Spek, 1990). The transmission-factor range is consistent with the range 0.13–1.00 as observed in  $360^\circ \psi$  scans. One lower-order reflection (012) was omitted from the final refinement cycles. A final difference density map did not show features other than residual absorption artifacts near Cs. The structure contains no residual solvent-accessible voids (Spek, 1994). Calculations were carried out on a DEC5000 cluster.

Data collection: locally modified *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *SET4* (de Boer & Duisenberg, 1984). Data reduction: *HELENA* (Spek, 1993). Program(s) used to solve structure: *SIR92* (Altomare, Cascarano, Giacovazzo & Guagliardi, 1993). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *PLATON* (Spek, 1990). Software used to prepare material for publication: *PLATON*.

This work was supported in part (ALS and NV) by the Netherlands Foundation of Chemical Research (SON) with financial aid from the Netherlands Organization for Scientific Research (NWO).

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Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: BR1107). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1995). **C51**, 1975–1977

## Czochralski-Grown SrLaGaO<sub>4</sub>

JAMES F. BRITTEN

*Department of Chemistry, McMaster University,  
1280 Main Street West, Hamilton, Ontario,  
Canada L8S 4M1*

HANNA A. DABKOWSKA, ANTONI B. DABKOWSKI  
AND JOHN E. GREEDAN

*Institute for Materials Research, McMaster  
University, 1280 Main Street West, Hamilton, Ontario,  
Canada L8S 4M1*

JOHN L. CAMPBELL AND WILLIAM J. TEESDALE

*Department of Physics, College of Physical and  
Engineering Science, University of Guelph, Guelph,  
Ontario, Canada N1G 2W1*

(Received 15 June 1994; accepted 17 October 1994)

## Abstract

The structure of Czochralski-grown lanthanum strontium tetraoxogallate, LaSrGaO<sub>4</sub>, a K<sub>2</sub>Ni<sub>2</sub>F<sub>4</sub>-type compound, has been redetermined by X-ray diffraction. The improved quality of the crystals resulted in a higher precision in the determination of the geometric parameters than reported previously [Rüter & Müller-Buschbaum (1990). *Z. Anorg. Allg. Chem.* **584**, 119–124]. La and Sr atoms are equally distributed on a nine-coordinate site, and Ga is in a distorted octahedral site stretched along [001]. PIXE analysis gives excellent quantitative results.

## Comment

Single crystals of SrLaGaO<sub>4</sub> have been structurally characterized. They are applicable as substrates for high-temperature superconducting thin films (McConnell *et al.*, 1994). The refined structure is in agreement with that published by Rüter & Müller-Buschbaum (1990) for submillimeter single crystals obtained by solid-state reaction; however, the improved quality and size of the crystals results in higher resolution data. There is about one order of magnitude improvement in the standard deviations of the bond lengths. For example, La—O1 is 2.428 (3) versus 2.42 (3) Å (Rüter & Müller-Buschbaum, 1990). A 50:50 distribution of La and Sr in the nine-coordinate site was assumed and confirmed by PIXE analyses (Johansson & Campbell, 1989). Ga occupies a distorted octahedral site. The O1 atom shows a higher  $U_{eq}$  value than atom O2 as a result of the significantly longer Ga—O1 distance.