THE CRYSTAL STRUCTURE OF THE TERNARY OXIDE 
Li2SiO4, by J.L. Perlov-Bialobrotn, M.E. Villa-
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Four stable new ternary compounds had been reported in the system Li2O-CaO-SiO2 (A.R. West, J. Am. Chem. Soc.
1978) but no crystal chemistry was done on them. We grew crystals of the Li2SiO4 phase of opti-
mum size for crystal structure analysis. Single crystal diffraction diagrams show the material to be tri-
clinic, P1, a = 10.4505(1)0027, b = 8.3125(0.0023), c = 
7.17600±0.0021, β = 77.17300.024, γ = 90.02504.023, γ = 109.249±0.022. The structure was solved using 2166 ob-
served reflections. Full matrix least squares refinement with anisotropic temperature factors was terminated 
when R = 0.038 and Rw = 0.041. In this structure the silicon in tetrahedral coordination forms two types of 
anions: a (SiO4) unit like a zig-zag chain, and a 
(SiO4) unit. The coordination polyhedra of the lithi-
um is also a tetrahedron, but distorted, and joins 
together the two silicon anions, forming two-dimensional 
layers. The calcium has a distorted cube-like coordina-
tion polyhedron that links the silicon-lithium layers.

08.2-23

08.2-24 COMPOUND FORMATION AND CRYSTAL CHEMISTRY IN 
THE SYSTEM Li2O - ZrO2 - SiO2, by Patricia Quintana,
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The new ternary compound Li2ZrSi6O15 has been found in the system 
Li2O - ZrO2 - SiO2, has a monoclinic unit cell of 
a = 11.121(6), b = 10.146(6), c = 11.235(7) Å, 
β = 100.26(5)° and space group P21/n. Its crystal 
structure appears to be closely related to that of Zekt-
zerite, Li2HfZr2Si11. In the system Li2O - ZrO2 
ine lithium zirconate phases have been prepared, five of which are new. One of the 
new phases is a high temperature polymorph of Li2ZrO3 
and the others are metastable phases. The thermal 
behaviour and reaction pathways of formation of the new 
phases were studied and their X-ray powder patterns are 
reported.

08.2-25 CRYSTAL STRUCTURES OF SOME METAL SACCAR-
INATO-HEREDS, by G. Jovanovski and B. Kamenar, Faculty of 
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The crystal structure of sodium saccharinato 2/3 hydrated (1), magnesium disaccharinato heptahydra-
te (2), tetraaquadisaccharinatoanganese(II) di-
hydrate (3), and disaccharinatomercury(II) (4) have been examined by X-ray analysis based on 
the intensity data collected on an automatic dif-
fractometer. In structure (1) two Na+ ions have 
C.N. six being surrounded by O atoms from water 
molecules, CO and SO4 groups from sacchari-
nates, the third Na+ ion has also C.N. six but 
realized by five O atoms from the same groups and 
by one saccharinato N atom. The Na to O distances 
range from 2.30 to 2.42 Å. In structure (2) a disacchari-
notered ion is octahedrally surrounded by five O atoms from wa-
ter molecules and one O atom from CO group. The 
Mg to O distances range from 2.05 to 2.11.3 Å. In 
(3) Na+ atom is in the centre of symmetry and has 
octahedral coordination being bonded to four wa-
ter-oxygen atoms and two saccharinato-nitrogen 
atoms. The Mn-O distances are 2.16.2 (2x) and 
221.9 (2x), while Mn-N amounts to 228.1 μ (2x). 
In the unit cell of (4) there are two independent 
molecules, both with digonal characteristic coordi-
nation of Mg atom. In one the Mg-O bond len-
ths are 203.5, 205.0 Å, while in the other 
202.9 and 205.8 Å, respectively. The Mg-N angles 
are 167.0° and 175.6°, respectively. In (1), (2) and (3) water molecules participate in hydro-
gen bonding with saccharinate ions. The sacchari-
nate ions are planar with bond lengths and angles 
within expected values. The structures have been 
refined to R values of (1) 0.039, (2) 0.038, 
(3) 0.028 and (4) 0.062.

08.2-26 MERCURY(II) COMPOUNDS WITH HIGH COORDI-
NATION NUMBERS, by K. Aurivillius and C. Stilstadste, 
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In mercury(II) compounds two-coordination is prevalent. In the coordination to O, Hg is in most cases linearly 
or almost linearly bonded at the short distances 2.0-2.2 Å. There are, however, often 3-5 more ligands at 2.4-2.9 Å, 
implying considerable weaker interactions. Four- and 
six-coordination for Hg(II) are rather unusual and coor-
dination numbers higher than six have so far been re-
ported only for K3[\(\text{Hg(N}_0\text{}_2\text{)}_4\text{]NO}_3\text{]} (Hall & Holland, Inorg.
Nucl. Chem. Lett. (1972) 8, 809, containing [\(\text{Hg(NO}_0\text{)}_2\text{]}^2\text{] ions. The eight oxygen atoms of the four nitrite groups form a 
highly distorted square antiprism around Hg with Hg-O 
bond lengths of 2.39-2.57 Å; the average value is 2.48 Å. 
Eight-coordinated Hg has now also been found in the two 
Hg(II) bromates [\(\text{Hg(BrO}_3\text{)}_2\text{]}_2\text{] and K\(\text{Hg(BrO}_3\text{)}_2\text{]}_2\text{] (Fig. 1).} 
A preliminary X-ray study of \(\text{Hg(BrO}_3\text{)}_2\text{]}_2\text{] has shown that 
Hg is bonded to two water molecules [Hg-Ow 2.35-2.34 Å] 
and four bromate groups [Hg-O 2.62-2.72 Å (Fig. 1)] by 
the average Hg-O bond being 2.48 Å. A neutron diffraction 
study is planned and the result will be presented at 
the congress.

In [\(\text{K}_3\text{Hg(BrO}_3\text{)}_2\text{]}_2\text{] the eight-coordination for Hg(II) 
is obtained by bonds to two nitrate [Hg-O 2.52-2.59 Å] 
and four bromate groups [Hg-O 4x2.43 Å (Fig. 1)] with 
an average Hg-Bond length of 2.50 Å.