08.2-23 THE CRYSTAL STRUCTURE OF THE TERNARY OXIDE Li$_2$Zr$_2$Si$_6$O$_{13}$ By L.E. Herdon-Dulles, A.M. Villa-Fuerte-Castrejon, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma, Mexico D.F., and C. Campana, Nicolet XRD Corp., Cupertino, CA 95014, U.S.A.

Four stable new ternary compounds had been reported in the system Li$_2$O-CaO-SiO$_2$ (A.R. West, J. Am. Gemm. Soc. 1978, 61, No. 3-4) but no crystal chemistry was done on them. We grew crystals of the Li$_2$Ca$_2$Si$_6$O$_{13}$ phase of optimum size for crystal structure analysis. Single crystal diffraction diagrams show the material to be triclinic, $P_1$, $a = 10.453(3)$, $b = 8.231(2)$, $c = 7.170(3)$, $\alpha = 77.71(2)$, $\beta = 90.02(2)$, $\gamma = 109.26(2)$. The structure was solved using 2166 observed reflections. Full matrix least squares refinement with anisotropic temperature factors was terminated when $R = 0.038$ and $R_p = 0.041$. In this structure the silicon in tetrahedral coordination forms two types of anions: a (Si$_4$O$_8$) unit like a zig-zag chain, and a (Si$_6$O$_{18}$)$^{2-}$ unit. The coordination polyhedra of the lithium is also a tetrahedron, but distorted, and joins together the two silicon anions, forming two-dimensional layers. The calcium has a distorted cube-like coordination polyhedron that links the silicon-lithium layers.

08.2-24 COMPOUND FORMATION AND CRYSTAL CHEMISTRY IN THE SYSTEM Li$_2$O - Zr$_2$O$_2$ - SiO$_2$. By Patricia Quintana, Universidad Nacional Autonoma de Mexico, División de Estudios de Posgrado, Facultad de Química, Ciudad Universitaria, Mexico 20, D.F., Mexico and Anthony R. West, Chemistry Dept., Aberdeen University, Meston Walk, Old Aberdeen, Scotland, Great Britain.

The new ternary compound Li$_2$ZrSi$_6$O$_{13}$, found in the system Li$_2$O - Zr$_2$O$_2$ - SiO$_2$, has a monoclinic unit-cell of dimensions $a = 11.121(6)$, $b = 10.146(6)$, $c = 11.235(7)$ A, $\beta = 100.28(5)^\circ$ and space group $P2_1/n$. Its crystal structure appears to be closely related to that of Zektzerite, Li$_6$Zr$_2$Si$_6$O$_{13}$. In the system Li$_2$O - Zr$_2$O$_2$ nine lithium zirconate phases have been prepared, five of which are new. One of the new phases has a high temperature polymorph of Li$_2$ZrO$_2$ 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 SACCHARINATES. By G. Jovanović and S. Ramanan, Faculty of Chemistry, University of Skopje and Faculty of Science, University of Zagreb, P.O. Box 153, 41001 Zagreb, Yugoslavia.

The crystal structure of sodium saccharinate 2/3 hydrate (1), magnesium disaccharinatoheptahydrate (2), tetraaquasaccharinatoanesthesia(II) dihydrate (3), and disaccharinato mercury(II) (4) have been examined by X-ray analysis based on the intensity data collected on an automatic diffractometer. In structure (1) two Na$^+$ ions have C.N. six being surrounded by 0 atoms from water molecules, CO and $\text{SO}_4$ groups from saccharinates, the third Na$^+$ ion has also C.N. six but realized by five O atoms from the same groups and by one saccharinate N atom. The Na to O distances vary from 230.4 to 240.5 pm. In one of the (4) water molecules is octahedrally surrounded by five O atoms from water molecules and one O atom from CO group. The Mg to O distances range from 183.0 to 221.9 pm. In (3) Na atom is in the centre of symmetry and has octahedral coordination being bonded to four water-oxygen atoms and two saccharinate-nitrogen atoms. The Mg-O distances are 216.2 (2x) and 221.9 (2x), while Mn-N amounts to 228.1 pm (2x). In the unit cell of (4) there are two independent molecules, both with digonal characteristic coordination of Hg atom. In one the Hg-N bond lengths are 202.9 and 205.0 pm, while in the other 202.9 and 205.8 pm, respectively. The M-Hg-N angles are 167.0 and 175.4°, respectively. In (1), (2) and (3) water molecules participate in hydrogen bonding with saccharinate ions. The saccharinate ions are planar with bond lengths and angles within expected values. The structures have been refined to $R$ values of (1) $0.039$, (2) $0.028$, (3) $0.028$ and (4) $0.062$.

08.2-26 MERCURY(II) COMPOUNDS WITH HIGH COORDINATION NUMBERS. By K. Aurivillius and C. Stihlande, Inorganic Chemistry, Chemical Center, University of Lund, P.O. Box 118 210 07 Lund, Sweden.

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 coordination numbers higher than six have so far been reported only for K$_3$[Hg(NO$_2$)$_4$]NO$_3$(Hall & Holland, Inorg. Chim. Acta 1969, 3, 235; Powar at al, Inorg. Chim. Acta 1969, 3, 235; Powar at al, Inorg. Nucl. Chem. Lett. 1972, 8, 809), containing [Hg(NO$_2$)$_4$]$_2$- ions. The eight oxygen atoms of the four nitrite groups form a highly distorted square antiprism around Hg with Hg-O bonds 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 Hg(BrO$_3$)$_2$·2H$_2$O and K$_3$Hg(BrO$_3$)$_2$(NO$_3$)$_2$. A preliminary X-ray study of Hg(BrO$_3$)$_2$·2H$_2$O has shown that Hg is bonded to two water molecules [Hg-O = 2.35, 2.34 Å] and four bromate groups [Hg-O 2.62-2.72 Å] (Fig. 1); 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 K$_3$Hg(BrO$_3$)$_2$(NO$_3$)$_2$ the eight-coordination for Hg(II) is obtained by bonds to two nitrate [Hg-O = 4x2.58 Å] and four bromate groups [Hg-O 4x2.43 Å] (Fig. 1) with an average Hg-O bond length of 2.50 Å.