08.2-23  THE CRYSTAL STRUCTURE OF THE TERNARY OXIDE Ll2O-Si2O5 by L. E. Berkton-Dubbintron, M. E. Villa- Fuerte-Castricen, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma, Mexico 20 D.F., and C. Campana, Nicolet XRQ Corp., Cupertino, CA 95014, U.S.A.

Four stable new ternary compounds had been reported in the system Li2O-CaO-SiO2 (A.R. West, J. Am. Ceram. Soc. 1978, 61, No. 3-4) but no crystal chemistry was done on them. We grew crystals of the Li2Ca4Si4O13 phase of optimum size for crystal structure analysis. Single crystal diffraction diagrams show the material to be triclinic, P1, a = 10.450(3), b = 8.312(3), c = 7.170(3) Å, $\beta = 77.713(2)^\circ$, $\gamma = 90.256(4)^\circ$, $\alpha = 108.269(2)^\circ$. The structure was solved using 7166 observed 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)2- unit like a zig-zag chain, and a (SiO4)63- 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 Li10 - ZrO2 - SIO2 by Patricia Quintana, Universidad Nacional Autonoma de Mexico, Division de Estudios de Posgrado, Facultad de Quimica, Ciudad Universitaria, Mexico 20, D.F., Mexico and Anthony R. West, Chemistry Dept., Aberdeen University, Montev Park, Old Aberdeen, Scotland, Great Britain.

The new ternary compound L12ZrSi5O15, found in the system Li10 - ZrO2 - SiO2, has a monoclinic unit-cell of dimensions a = 11.121(6), b = 10.114(6), c = 11.235(7) Å, $\beta = 100.26(5)^\circ$ and space group P21/n. Its crystal structure appears to be closely related to that of Zektzerite, L12Ca2Zr5O15.

In the system Li10 - ZrO2 nine 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 SACCHARINATES by G. Jovanovski and B. Kamenar, Faculty of Science, University of Zagreb, P.O. Box 135, 41001 Zagreb, Yugoslavia.

The crystal structure of sodium saccharinate 2/3 hydrate (1), magnesium disaccharinate heptahydrate (2), tetraaquasaccharinatomanganese(II) dihydrate (3), and disaccharinotetraorganometallic(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, five water molecules, CO and SO 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 saccharinato N atom. The SO2 to O distances range from 230.4 to 279.6 pm and seven O atoms from water molecules and one O atom from CO group. The Mg2+ to O distances range from 203.0 to 211.3 pm. In (3) Mn atom is in the centre of symmetry and has octahedral coordination being bonded to four water-oxygen atoms and two saccharinato-nitrogen atoms. The Mn-O distances are 215.2 (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 atoms. In one the Hg-O bond lengths are 203.8 and 205.0 pm, while in the other 202.9 and 205.8 pm, respectively. The Hg-Mg angles are 167.0 and 175.6°, respectively. In (1), (2) and (3) water molecules participate in hydrogen bonding with saccharinate ions. The saccharinate ions planar with bond lengths and angles within expected values. The structures have been refined to R values of (1) 0.029, (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. Stenhandske, Inorganic Chemistry, Chemical Center, University of Lund, P.O. Box 740, 22100 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 K3[Hg(NO3)3]NO3·H2O (Hull & Holland, Inorg. Chim. Acra, 1969, 3, 235; Powar at al., 1970) and for five nitrate groups with Hg(II) from dimers 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(BrO3)2·2H2O and Hg3[BBrO3]2(NO3)2. A preliminary X-ray study of Hg(BrO3)2·2H2O has shown that Hg is bonded to two water molecules [Hg-Ow 2.35,2.34 Ä] and four bromate groups [Hg-O 2.52-2.72 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 K3Hg(BrO3)2(NO3)2 the eight-coordination for Hg(II) is obtained by bonds to two nitrate [Hg-O 2.35,2.59 Å] and four bromate groups [Hg-O 2.42-2.43 Å] (Fig. 1) with an average Hg-O bond length of 2.50 Å.
There also exist analogous Cd compounds with the compositions Cd(BrO$_3$)$_2$·2H$_2$O (Hurtý & Hurtý, Z. Kristallogr. 1978 164, 10) and K$_2$Cd(BrO$_3$)$_2$·(SO$_4$)$_2$. We have found that Cd(BrO$_3$)$_2$·2H$_2$O is isomorphous with K$_2$(BrO$_3$)$_2$·2H$_2$O and that K$_2$Cd(BrO$_3$)$_2$·(SO$_4$)$_2$ has most probably a structure very similar to that of the K$_2$-compound. The cell dimensions are close to those of K$_2$Cd(BrO$_3$)$_2$·(SO$_4$)$_2$ but the space group has changed from P2$_1$/m to P2$_1$/n.

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08.2-28 STRUCTURE DETERMINATION OF Li$_2$Pt$_3$O$_7$ AND Co$_2$Na$_5$Pt$_3$O$_{14}$ BY NEUTRON POWDER DIFFRACTION. By K.B. Schwartz, J.B. Parish, Department of Earth and Planetary Sciences, SUNY, Stony Brook, New York, and R.D. Shannon, Central Research and Development, E.I. du Pont de Nemours and Company, Wilmington, Delaware, USA.

Li$_2$Pt$_3$O$_7$, a member of the Na$_2$Pt$_3$O$_7$ structural family (Bürger and Kohlhass, Z. Anorg. Allg. Chem. 1973 401, 15), has been synthesized by solid state reaction of Li$_2$CO$_3$, LiOH, and CuPt. Refinement of neutron powder diffraction data by profile analysis (Rietveld, J. Appl. Cryst. 1969 2, 65) has determined that Li$_2$Pt$_3$O$_7$ is not isomorphic with Na$_2$Pt$_3$O$_7$ (space group P2$_1$/n) but belongs to the acentric subgroup P2$_1$. Li$_2$Pt$_3$O$_7$ has unit cell dimension a=6.524 Å, contains Li in position 2a (0,0,0), Pt in position 6d (1/4,1/4,1/4) and O in position 8e (x,x,x) with x=0.2720(3). Equivalent isotropic temperature factors for Li, Pt and O are 2.8(6), 0.11(4) and 0.95(4), respectively. The structure is distinguished by distortion of the cubic coordination polyhedron about Li to two interpenetrating tetrahedra with Li-O distances of 2.22 Å and 2.65 Å. Pt coordination remains square-planar with a slight tetrahedral distortion and a Pt-O distance of 2.00 Å. Refinement of scattering power on the Li site yields a Li occupancy of 0.67(5) atoms per formula unit, in close agreement with chemical analysis (0.64(1) by atomic absorption). Final discrepancy factors for this refinement are R=0.06, Rm=0.10 and R=0.15,94. Co$_2$Na$_5$Pt$_3$O$_{14}$, with a=4.00 Å and y=0.11 as determined by atomic absorption, was synthesized by solid state reaction of CoPt$_3$, NaF, and Co(NO$_3$)$_2$·6H$_2$O and CuPt. Neutron powder diffraction experiments have indicated the presence of reflections of the type hhl: 12/2, in violation of both space groups Pn2$_1$ and Pn. This reduction in symmetry is a result of ordering of Co and Na on distinguishable eight-coordinated sites. Co$_2$Na$_5$Pt$_3$O$_{14}$ belongs to a subgroup of Pn2$_1$ with the centric Pn3 or the acentric Pn2$_1$. Both these space groups are characterized by Oddo ordering of Co and Na in the ratio 1/2,1/2,1/2 unrelated by symmetry, which is compatible with ordering of Co and Na.