

Abstracts of Forthcoming Articles

La structure Pb_3ZrF_{10} : Base pour deux nouvelles séries homologues de phases ordonnées dérivant de la fluorine par excès d'anions. B. FRIT* AND J. P. LAVAL, Laboratoire de Chimie Minérale Structurale, Université de Limoges, 123, rue Albert Thomas, 87060 Limoges Cédex, France. Examination of the fluorite-related Pb_3ZrF_{10} structure revealed that anion excess is localized within infinite columns of independent square antiprisms [ZrF_6]. This monodimensional B_2X_8 cluster, formed in other known anion-excess fluorite-related superstructures, can be used as a basic structural unit for an original homologous series, formulated $A_nB_2X_{2n+8}$ ($n \geq 2$), or more generally M_mX_{2m+4} , whose compounds $BaZrF_{6\alpha}$ ($n = 2$, highly distorted), K_2ReF_8 ($n = 4$), Pb_3ZrF_{10} ($n = 6$), and probably Pb_5ZrF_{14} ($n = 10$) are the first known members. Another new homologous series $A_nB_2X_{2n+6}$ or M_mX_{2m+2} with an infinite column B_2X_6 of independent [BX_7] polyhedra as the basic structural unit is proposed. K_2NbF_7 is described as the member $n = 4$ of this series, whose compounds Pb_3TiF_9 , $Ba_9Al_2F_{24}$ and Pb_5GaF_{13} could be the members respectively $n = 6, 9, 10$. It is shown that monodimensional-cluster models can be used successfully for the description of any anion-excess fluorite-related compounds exhibiting cations with wide difference in size.

The 1-6 Weberite $Na_2Te_2O_7$ and Some Observations on Compounds with the Weberite Structure. O. KNOP* AND G. DEMAZEAU, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia B3H 4J3, Canada. The 1-6 weberite $Na_2Te_2O_7$ ($Imm2$, $a = 7.233 \text{ \AA}$, $b = 10.104 \text{ \AA}$, $c = 7.454 \text{ \AA}$) has been prepared by high-pressure synthesis. It is shown that \bar{a} (the mean unit-cell dimension per formula unit) of oxide weberites $A_2B_2O_7$ can be represented as a linear function of the effective ionic radii of A and B. The problem of the true space-group symmetry of weberite is discussed.

The Crystal Structure of hcc-CuAsSe. H. J. WHITFIELD, CSIRO Division of Chemical Physics, P.O. Box 160, Clayton, Victoria, Australia 3168. The crystal structure of synthetic copper selenide, CuAsSe, has been determined by a three-dimensional single-crystal X-ray examination using film data. The crystals, of orthorhombic space group $Pbcn$, have $Z = 24$ in a unit cell of dimensions $a = 11.75 \pm 0.02$, $b = 6.79 \pm 0.01$, and $c = 19.21 \pm 0.03 \text{ \AA}$. The structure was solved by Patterson projection and electron density methods and isotropically refined to $R = 0.125$ for 300 observed reflections. The structure of CuAsSe is related to the $B6$ structure of $6H$ ZnS as CuAsS is to the $B3$ structure of zincblende. Alternately, in Jagodzinski nomenclature, CuAsSe has hcc packing rather than ccc packing of CuAsS.

Preparation of New Crystal Form of Manganese Dioxide: λ - MnO_2 . J. C. HUNTER, Union Carbide Corporation, P.O. Box 6116, Cleveland, Ohio 44107. Treatment of the spinel-type material $LiMn_2O_4$ with aqueous acid was found to result in conversion of the $LiMn_2O_4$ to nearly pure MnO_2 while preserving the structural framework of the $LiMn_2O_4$. The resulting material, designated λ - MnO_2 , thus has a structure related to spinel, but with most of the lithium removed from the tetrahedral sites. The conversion of $LiMn_2O_4$ to λ - MnO_2 results in some contraction of the lattice, as evidenced by a reduction in the lattice constant a_0 from 8.24 to 8.03 \AA . A mechanism for the conversion of $LiMn_2O_4$ to λ - MnO_2 is proposed, which involves solid state diffusion of lithium in the structure, in a manner analogous to the proton diffusion which occurs during the cathodic reduction of γ - MnO_2 .

EPR Detection of Acetate Ions Trapping in B-Type Carbonated Fluorapatites. G. BACQUET,* V. Q. TRUONG, M. VIGNOLES, AND G. BONEL, Laboratoire de Physique des Solides, Associé au CNRS, 118, Route de Narbonne, 31062 Toulouse Cédex, France. Carbonated fluorapatites were prepared by precipitation using calcium acetate. After irradiation and annealing at 150°C the X-band ESR spectrum of the CH_3 radical was recorded. The spin Hamiltonian parameters were determined at RT, 110 K, and 16 K. From the thermal behavior of the spectrum it is deduced that different recombination processes of the defect are involved. This radical originates from the degradation of acetate ions trapped at anion sites of the tunnels.

Note. Asterisks indicate authors to be addressed.