JOURNAL OF SOLID STATE CHEMISTRY 14, 112–115 (1975)

Abstracts of Forthcoming Articles

Crystal Growth and Electrical Conduction of $PbMoO_4$ and $PbWO_4$. W. VAN LOO. Solid State Chemistry Department, Physical Laboratory, State University, Utrecht, The Netherlands. The phenomenon of the colouration of Czochralski-grown single crystals of $PbMoO_4$ and $PbWO_4$ is discussed. This colouration is supposed to be related with an intrinsic point defect. We propose that during the crystal growth a loss of oxygen occurs and consequently, oxygen deficient crystals are produced. The existence of electronic charge carriers at high temperatures and ionic majority defects in the oxygen sublattice is confirmed by conductivity measurements. The colour center is supposed to be an oxygen vacancy which has trapped one or two electrons. On the basis of this simple model various aspects of the colouration can be understood.

The Crystal Structure of Cobalt Orthophosphate, $Co_3(PO_4)_2$. J. B. ANDERSON, E. KOSTINER, M. C. MILLER, AND J. R. REA. Institute of Materials Science, University of Connecticut, Storrs, Connecticut 06268. The crystal structure of cobalt orthophosphate has been refined by full-matrix least-squares procedures using automatic diffractometer data to a residual $R = 0.039$ ($R_w = 0.058$). The space group is $P2_1/c$, with $a = 5.064(3)$, $b = 8.365(4)$, $c = 8.794(4)$ Å and $\beta = 120.98(3)°$. $Co_3(PO_4)_2$ is isotypic with the previously reported γ-$Zn_3(PO_4)_2$ and $Mg_3(PO_4)_2$. Cobalt ions occupy two distinct coordination polyhedra, one five- and one six-coordinated, in a ratio of two to one. The structure is described in detail.

Structural Studies of Some Body-Centered-Cubic Phases of Mixed Oxides Involving Bi_2O_3. The Structures of $Bi_{25}FeO_{40}$ and $Bi_{38}ZnO_{60}$. D. C. CRAIG AND N. C. STEPHENSON. School of Chemistry, University of New South Wales, Kensington, N.S.W., Australia. The structures of the compounds initially reported to be $7.Bi_2O_3 \cdot ZnO$ and $96.Bi_2O_3 \cdot 4Fe_2O_3$, have been determined by X-ray methods. Three-dimensional absorption corrected diffractometer data were used and atomic parameters were refined by least-squares procedures. The structures are isomorphous, cubic with $a =$ 10.194 (3) and 10.179 (3) Å, respectively, and space group $I23$. Each Bi^{3+} ion is surrounded by five oxygen atoms which form an incomplete octahedral arrangement with Bi–O distances ranging from 2.07 to 2.60 Å. The $6s^2$ inert electron pair completes the octahedron. The Bi^{3+} ions are vibrating anisotropically. Tetrahedral sites in the structures contain 61 and 46 electrons, respectively. These values are consistent with a statistical distribution of Zn^{2+} and Bi^{5+} ions or Fe^{3+} and Bi^{5+} ions on these sites. Molar ratios are derived which agree with the observed distributions of electron density and also give rise to perfectly stoichiometric systems, devoid of cationic or anionic vacancies. The compositions studied correspond to $Bi_{24}^{3+}Bi^{5+}Fe^{3+}O_{40}$ and $Bi_{36}^{3+}Bi_2^{5+}ZnO_{60}$ and they are optical enantiomorphs. It is proposed that a reduction in the percentage composition of Bi_2O_5 leads to metastable phases, in which all atomic positions remain fully occupied but some tetrahedral sites contain Bi^{3+} ions. The end product of the series is γ-Bi_2O_3 in which 50% of these sites contain Bi^{3+} and the remainder Bi^{5+} ions. We believe that γ-Bi_2O_3 is $Bi_{25}^{+3}Bi^{+5}O_{40}$.

Magnetic Property in the System $BaCo_{1-x}Ni_xO_3$ ($x = 0 \sim 1$). Y. TAKEDA. The Institute of Scientific and Industrial Research, Osaka University, Osaka 565, Japan. The system of $BaCo_{1-x}Ni_xO_3$ ($x = 0 \sim 1$) with a two-layer hexagonal perovskite-type structure are prepared at an oxygen pressure of 2000 bar. The change in unit cell parameters is not linear. Magnetic measurements indicate that $BaCoO_3$, $BaCo_{0.9}Ni_{0.1}O_3$, and $BaCo_{0.8}Ni_{0.2}O_3$ are antiferromagnetic with $T_N = 8, 10$, and 10 K respectively.

Interstitial Superstructures in the Ta–D System. H. ASANO, Y. ISHINO, R. YAMADA, AND M. HIRABAYASHI. The Research Institute for Iron, Steel and Other Metals, Tohoku University, Sendai 980, Japan. Ordered deuterium arrangements and order–disorder transformations of the tantalum deuterides in the range $TaD_{0.50}$–$TaD_{0.78}$ have been studied by neutron diffraction and calorimetry at temperatures between −170 and 120°C. In addition to the disordered phase (α), are clarified three ordered phases based on the superstructures $Ta_2D_{1+x}(\beta_1)$, $Ta_4D_3(\gamma)$ and $TaD(\delta)$. The

Printed in Great Britain