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Abstracts of Forthcoming Articles

Neutron Powder Diffraction and Magnetic Measurements on $RbTiI_3$, $RbVI_3$, and $CsVI_3$. H. W. ZANDBERGEN, Gorlaeus Laboratories, University of Leiden, P.O. Box 9502, 2300 RA Leiden, The Netherlands. $CsVI_3$ (a = 8.124(1), c = 6.774(1) Å, Z = 2, $P6_3/mmc$ at 293 K) adopts the $BaNiO_3$ structure. Three-dimensional magnetic ordering takes place at T_c = 32(1) K. At 1.2 K the magnetic moment is 1.64(5) μ_B and it forms a 120° spin structure in the basal plane. $RbVI_3$ (a = 13.863(2), c = 6.807(1) Å, Z = 6, $P6_3cm$ or $P\bar{3}c1$ at 293 K) and $RbTiI_3$ (a = 14.024(3), c = 6.796(2) Å, Z = 6, $P6_3cm$ or $P\bar{3}c1$ at 293 K) adopts a distorted $BaNiO_3$ structure, probably isostructural with $KNiCl_3$. T_c of $RbVI_3$ is 25(1) K. At 1.2 K, $RbVI_3$ has a spin structure similar to the one of $CsVI_3$ with a magnetic moment of 1.44(6) μ_B. $RbTiI_3$ shows no magnetic ordering at 4.2 K. It is shown that a deviation from the 120° structure is expected for compounds with a distorted $BaNiO_3$ structure such as $RbVI_3$. The cell dimensions of $CsTiI_3$ are reported.

The Resistivity and Magnetic Susceptibility of V_3O_5 Single Crystals. H. JHANS AND J. M. HONIG,* Department of Chemistry, Purdue University, West Lafayette, Indiana 47907. New resistivity studies on single-crystal V_3O_5 show that the phase transformation at 427 K involves an insulator–metal transition; the resistivities reported here lie somewhat below those cited in numerous earlier investigations. Magnetic susceptibility (χ) measurements exhibit only very small changes at the transition. It is pointed out that the maximum in χ at 125 K should be correlated with the onset of antiferromagnetic ordering near 76 K.

Forces de la Liaison Te–O: Coordination et Localisation de la Paire Libre de l'Atome de Tellure IV dans les Tellurites. E. PHILIPPOT, Laboratoire de Chimie Minerale C, Université des Sciences et Techniques du Languedoc, Place Eugene Bataillon, 34060 Montpellier, France. The calculation of bond valences (S) from the bond lengths (R) observed in many accurate structure determinations of tellurites, Te^{IV}, using the relation $S = S_0(R/R_0)^{-N}$, allows us to refine the R_0 and N values proposed by Brown. If we classify the different TeO_y surroundings by taking into account the three strongest bond valences in their relation to the weakest one, it can be verified that the observed variation allows us to foresee the atomic coordination of tellurium IV atom with respect to the other components of the structure. On the other hand, the probable location of the lone pair $5s^2$ of tellurium IV atom can be related to the evolution of its coordination.

Bidimensional Magnetic Properties of β-Sr_2MnO_4. J. C. BOULOUX, J. L. SOUBEYROUX, G. LE FLEM,* AND P. HAGENMULLER, Laboratoire de Chimie du Solide, Universite de Bordeaux I, 351 cours de la Liberation, 33405 Talence, France. β-Sr_2MnO_4 belongs to the K_2NiF_4-type structure. The magnetic structure studied by neutron diffraction is characterized by antiferromagnetic interactions between nearest-neighbor Mn^{4+} ions. The value of the exchange integral J/k calculated by the high-temperature series expansion method is about −80 K. All magnetic properties of β-Sr_2MnO_4 show the two-dimensional character of the magnetic interactions and illustrate the strong covalency of the Mn–O bonds within the magnetic layers.

Le Système $BaFeO_{2.50}$–$BaZnO_2$.II. Conductivité Mixte et Autres Propriétés Physiques. P. NEU, M. ZANNE, C. GLEITZER,* AND G. DUDLEY, Laboratoire de Chimie du Solide Minéral, Université de Nancy I, 54037 Nancy, France. The α phase, perovskite type, $BaFe_{1-x}Zn_xO_{2.5-x/2}$ ($0.05 < x < 0.40$), shows weak ferrimagnetism for $x < 0.25$, with T_c around 470°C, and paramagnetism (above 77 K) for $x > 0.25$, which means progressive destruction of the antiferromagnetic order observed in $BaFeO_{2.5}$. The β ($Ba_4Fe_2Zn_2O_9$) and γ ($BaZn_{1-y}Fe_yO_{2+y/2}$) phases present properties in agreement with a strong perturbation of the perovskite octahedral site. The electrical conductivity is rather high, of mixed character, with a differing ionic–electronic distribution, depending on the synthesis conditions and on the temperature, due to different activation energies. The oxygen diffusion

Note. Asterisks indicate author to be addressed.

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coefficient which can be deduced is high, but the carrier number is limited through formation of vacancy pairs tending to give 4 coordination for iron.

Surface Instability and Nonstoichiometry of α-Fe_2O_3. J. H. W. DeWit,* A. F. Broersma, and M. Stroband, Inorganic Chemistry Department, University of Utrecht, Croesestraat 77A, 3522 AD Utrecht, The Netherlands. The thermodynamic stability region of α-Fe_2O_3 is investigated by thermogravimetric measurements. By means of electron microscopy, the surface of the grains of sintered compacts is shown to be already reduced well within the α-Fe_2O_3 stability region. Based on this information an electrical conductivity model is presented, in which the inhomogeneous character of the nonstoichiometry of the grains is emphasized.

Mössbauer Studies of Thiospinels.III. The System $FeCr_2S_4$–$FeIn_2S_4$. E. Riedel* and R. Karl, Institut für Anorganische und Analytische Chemie, Technische Universität Berlin, D-1000 Berlin 12, Germany. Polycrystalline samples of spinel compounds $FeCr_{2-x}In_xS_4$ have been obtained in the range $0 \leq x \leq 2$. The nonlinear changes of the cell parameters are explained by the nonlinear behavior of the inversion parameter λ according to the ionic distribution $Fe^{2+}_{1-\lambda}In^{3+}_{\lambda}[Cr^{3+}_{2-x}Fe^{2+}_{\lambda}In^{3+}_{x-\lambda}]S^{2-}_4$. Room-temperature ^{57}Fe-Mössbauer spectra exhibit two sets of absorptions for tetrahedrally and octahedrally coordinated Fe, respectively, each consisting of several overlapping doublets of similar isomer shifts but varying quadrupole splittings. The partial intensity of octahedral site Fe is in agreement with λ. The spectra can be understood by accounting for the influence of variable octahedral-site neighbors on tetrahedral-site iron.

Mössbauer Studies of Thiospinels.IV. The System $FeCr_2S_4$–Fe_3S_4. E. Riedel* and R. Karl, Institute für Anorganische und Analytische Chemie, Technische Universität Berlin, D-1000 Berlin 12, Germany. Spinel compounds of the composition $Fe_{1+x}Cr_{2-x}S_4$ with $0 \leq x \leq 0.5$ have been prepared in polycrystalline form. The ionic distribution $Fe^{2+}[Cr^{3+}_{2-x}Fe^{3+}_x]S^{2-}_4$ is derived from both X-ray and ^{57}Fe-Mössbauer data. Room-temperature Mössbauer spectra show the typical behavior of tetrahedral-site Fe^{2+} surrounded by different octahedral-site neighbors. Octahedral-site Fe^{3+} absorbs as a doublet with $\Delta \approx 0.5$ mm/sec. Samples of overall composition $FeCr_2S_4$ consist mainly of a spinel $Fe^{2+}[Cr^{3+}_{2-y}Fe^{3+}_y]S^{2-}_4$, $y \approx 0.02$.

Crystal Data and Phase Transitions of $KLiWO_4$ *and* $KLiMoO_4$. K. Okada* and J. Ossaka, Department of Inorganic Materials, Tokyo Institute of Technology, O-okayama, Meguro, Tokyo 152, Japan. Crystal data and phase transitions of $KLiWO_4$ and $KLiMoO_4$ were investigated using a high-temperature X-ray powder diffractometer. Phase transitions were observed at 350°C for $KLiWO_4$ and 360°C for $KLiMoO_4$. It was found that the room-temperature phases were isostructural with stuffed derivatives of tridymite and the high-temperature phases were isostructural with stuffed derivatives of cristobalite.

Champ de Force et Caracterisation des Liaisons dans Les Niobates et Tantalates de Structure de Type "Blocs 1 × 2." Y. Repelin,* E. Husson, and H. Brusset, Laboratoire de Chimie et Physico-Chimie Minerales, Institut de Chimie Ecole Centrale des Arts et Manufactures, 92290-Chatenay-Malabry, France. The vibrational study of the three families of the niobates and tantalates of "1 × 2 block"-type structure shows that some vibrational frequencies are characteristic of this structure. The relation between the calculated force constants and the structural characteristics permitted us to distinguish the different types of Nb–O and Ta–O bonds from each other, and to establish a relation between the polarizability of the divalent cation and the mode of linkage of the double octahedra in the layer planes. Finally, the comparison of these results with those obtained for other niobates and tantalates of various structures permitted us to determine the relative stability of all these compounds.

Phenomenological and Structural Study of a Low Temperature Phase Transition in the $PbZrO_3$–$PbTiO_3$ *System.* A. Amin,* R. E. Newnham, L. E. Cross, and D. E. Cox, Materials Research Laboratory, The Pennsylvania State University, University Park, Pennsylvania 16802. The Landau–Ginsburg–Devonshire Phenomenological theory has been applied to the $PbZrO_3$–$PbTiO_3$ crystalline solid solution system to explore the behavior of the rhombohedral:tetragonal morphotropic phase