

$\text{KTi}_2\text{Ta}_5\text{O}_{17}$ crystallizes in the orthorhombic system with unit-cell dimensions (from single-crystal data) $a=6.672(4)$ Å, $b=8.948(5)$ Å, $c=21.403(9)$ Å and space group $Cmcm$, $Z=4$. The structure was solved using three-dimensional Patterson and Fourier techniques. Of the 1034 reflections measured by counter techniques, 704 with $I \geq 3 \sigma(I)$ were used in the least-squares refinement of the model to a conventional R of 0.041 ($wR = 0.043$). The structure consists of edge- and corner-shared tantalum octahedra joined such that tunnels are formed in which the potassium ions are located. Slabs of octahedra are of the rutile (TiO_2) type related to one another by mirror planes (in which the potassium ions are located), producing a structure that may be considered as a "chemical twin" of the rutile structure.

An Experimental and Theoretical Study of Crystals of Calcium Fluoride Doped with Alkali Metal Cations. P. W. M. JACOBS S. H. ONG, A. V. CHADWICK, AND V. M. CARR. Department of Chemistry, University of Western Ontario, London, Ontario N6A 5B7, Canada.

Experimental measurements of thermal depolarization in crystals of CaF_2 , grown from the melt containing LiF, NaF, KF, or RbF, reveal a common relaxation (designated M_2) with an activation energy of 0.51 eV. In addition, the Li^+ - and K^+ -doped crystals exhibit a relaxation (M_1) with an activation energy of 0.34 eV. A similar relaxation has been found in $\text{CaF}_2:\text{Rb}^+$ and in $\text{CaF}_2:\text{Na}^+$. Theoretical calculations on M^+ -doped CaF_2 (where $M = \text{Li, Na, K, Rb}$) are in agreement with the hypothesis that the M_2 relaxation is due to Na^+ in all four systems studied and is associated with the jump of a nearest-neighbor (nn) anion vacancy (F_v^-) around the substitutional Na^+ ion (Na_s^+). The assignment of M_1 is less certain, but it appears to be associated with similar $\text{Li}_s^+ - \text{F}_v^-$ dipoles resulting from Li^+ impurity present because of the lower volatility of LiF compared to that of KF and RbF. When LiF dissolves in CaF_2 the Li^+ ion also forms quadrupoles consisting of a cation vacancy and two Li^+ interstitials and the reorientation of these quadrupoles has also been studied theoretically.

Defect Structures in the Brannerite-Type Vanadates. I. Preparation and Study of $\text{Mn}_{1-x}\phi_x\text{V}_{2-2x}\text{Mo}_{2x}\text{O}_6$ ($0 \leq x \leq 0.45$). ROMAN KOZŁOWSKI, JACEK ZIOLKOWSKI, KRZYSZTOF MOCALA, AND JERZY HABER. Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, ul. Niezapominajek, 30-239 Krakow, Poland.

Phases of the formula $\text{Mn}_{1-x}\phi_x\text{V}_{2-2x}\text{Mo}_{2x}\text{O}_6$ with the brannerite-type (α) structure, where ϕ_x represents a vacancy at a Mn site, have been synthesized and characterized by X-ray diffraction and DTA. The X-ray data are listed for MnV_2O_6 and solid solution with $x = 0.40$. They indicate random distribution of V and Mo over the original V sites and random distribution of Mn and vacancies over the original Mn sites. The monoclinic cell dilates with increasing x , primarily in the direction of the b -axis. The phase diagram of the pseudobinary $\text{MnV}_2\text{O}_6\text{-MoO}_3$ system has been determined. The extent of the stability region for the investigated brannerite solid solution has been established ($x_{\text{max}} = 0.45$ at 580°C). Other features determined in this system were: (a) little solubility of MoO_3 in the high-temperature (β) modification of MnV_2O_6 , (b) a two-phase area of α - and β -type solid solution coexistence, (c) a eutectic point between α -type solid solution and MoO_3 at 583°C and 75 mole% of MoO_3 , and (d) phase relationships at the liquidus.

Electric Properties of Ferromagnetic $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ ($0.5 \leq x \leq 0.9$). H. TAGUCHI, M. SHIMADA, AND M. KOIZUMI. The Institute of Scientific and Industrial Research, Osaka University, Suita, Osaka 565, Japan. The electrical resistivity of ferromagnetic $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ ($0.5 \leq x \leq 0.9$) was measured in the temperature range from 77 to 300 K. All cobaltites are good conductors and have a metallic coefficient. The magnetic transitions are independent of the electrical conductivity in this system. The logarithms of the specific electrical resistivities ($\log \rho$) at 80 and 290 K monotonically increase with mole fraction x , and these increases are explained by the itinerant-electron model.