

$\text{KTi}_2\text{Ta}_5\text{O}_{17}$  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 ( $\text{TiO}_2$ ) 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  $\text{CaF}_2$ , 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  $\text{Li}^+$ - and  $\text{K}^+$ -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  $\text{CaF}_2$  (where  $M = \text{Li, Na, K, Rb}$ ) are in agreement with the hypothesis that the  $M_2$  relaxation is due to  $\text{Na}^+$  in all four systems studied and is associated with the jump of a nearest-neighbor (nn) anion vacancy ( $F_v^-$ ) around the substitutional  $\text{Na}^+$  ion ( $\text{Na}_s^+$ ). The assignment of  $M_1$  is less certain, but it appears to be associated with similar  $\text{Li}_s^+ - F_v^-$  dipoles resulting from  $\text{Li}^+$  impurity present because of the lower volatility of LiF compared to that of KF and RbF. When LiF dissolves in  $\text{CaF}_2$  the  $\text{Li}^+$  ion also forms quadrupoles consisting of a cation vacancy and two  $\text{Li}^+$  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 ( $\alpha$ ) structure, where  $\phi_x$  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  $\text{MnV}_2\text{O}_6$  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  $580^\circ\text{C}$ ). Other features determined in this system were: (a) little solubility of  $\text{MoO}_3$  in the high-temperature ( $\beta$ ) modification of  $\text{MnV}_2\text{O}_6$ , (b) a two-phase area of  $\alpha$ - and  $\beta$ -type solid solution coexistence, (c) a eutectic point between  $\alpha$ -type solid solution and  $\text{MoO}_3$  at  $583^\circ\text{C}$  and 75 mole% of  $\text{MoO}_3$ , 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.