

*The Structure of Fluorides. X. Neutron Powder Diffraction Profile Studies of UF<sub>6</sub> at 193 and 293 K.* J. C. TAYLOR AND P. W. WILSON. Chemical Technology Division, Australian Atomic Energy Commission, Research Establishment, Sutherland, New South Wales, Australia, 2232. Neutron diffraction studies on polycrystalline UF<sub>6</sub> have been carried out at 193 and 293 K. At both temperatures, UF<sub>6</sub> is orthorhombic with the space groups  $Pnma(D_{2h}^{16})$  and  $Z = 4$ . Measured lattice parameters are  $a = 9.924(10)$  Å,  $b = 8.954(9)$  Å,  $c = 5.198(5)$  Å at 293 K, and  $a = 9.843(11)$ ,  $b = 8.920(10)$ ,  $c = 5.173(6)$  Å at 193 K. The neutron diffraction patterns were analysed by the least squares profile-fitting technique. The final values of  $R = \sum_i (|I_{o_i} - I_{e_i}|) / \sum I_{o_i}$  over the pattern points, where  $I_{o_i}$  is a background corrected measured intensity were 0.081 at 193 K and 0.133 at 293 K. On cooling, the hexagonal close packing tends to become more regular, and the F-F distances external to a UF<sub>6</sub> octahedron contract. The octahedra are nearly regular with a mean U-F distance of 1.98 Å, a mean F-F edge of 2.80 Å and F-U-F angle of 90.0° at 193 K.

*Chemical Hysteresis in Phase Transitions in the Terbium Oxide-Oxygen System.* A. T. LOWE AND L. EYRING. Department of Chemistry, Arizona State University, Tempe, Arizona 85281. A thermogravimetric study of hysteresis in the TbO<sub>x</sub>-O<sub>2</sub> system has provided insight into phase transitions occurring among the fluorite-related rare earth oxides. A series of isobaric scanning loops at 380 Torr have been made. The scans were between TbO<sub>1.5</sub>( $\phi$ ) and TbO<sub>1.714</sub>( $i$ ) at higher temperatures and between TbO<sub>1.174</sub>( $i$ ) and TbO<sub>1.818</sub>( $\delta$ ) at lower temperatures. Corresponding isobaric studies were made utilizing high temperature X-ray powder diffraction to augment the TGA (thermogravimetric analysis) experiments. It was confirmed that sections of the lower temperature loop were dependent on the rate of temperature change while the higher temperature loop was entirely reproducible. Interior scanning loops made within the lower hysteresis loop showed univariant behavior typical of a single phase when reversed in the  $\delta'$ - $\delta$  pseudophase region, otherwise it exhibited bivariant behavior. The upper hysteresis loop showed bivariant behavior throughout the interior of the loop. Some thermodynamic aspects and the microdomain concept as applied to hysteresis are also considered.

*Identification and Investigation of Impurities in Undoped Hg<sub>1-x</sub>Cd<sub>x</sub>Te.* JACOB W. LIN. Honeywell Corporate Research Center, 10701 Lyndale Avenue South, Bloomington, Minnesota 55420. The effect of impurities on electrical properties has been one of the most informative uses for the well-known infrared sensing material mercury-cadmium telluride. The relationship between the excess holes ( $p$ -type) or excess electrons ( $n$ -type) of undoped mercury-cadmium telluride Hg<sub>1-x</sub>Cd<sub>x</sub>Te ( $0.23 \approx x \approx 0.4$ ) and the residual impurities in the crystals were investigated. The impurities in the undoped material were determined using emission spectrometry, atomic absorption, and spark source mass spectrometry. Trace analysis indicates that impurities such as Cu and Ag consistently appear in  $p$ -type samples. Although these elements are not frequently observed in  $n$ -type substance, occasionally they are found in the material in a minute amount. Impurities such as Si, Cr, Pb, Li, Rb, Co, and Sn have been detected in both  $p$ -type and  $n$ -type materials. The possible correlation of these impurities with the  $p$ -type or  $n$ -type behavior of the undoped material is discussed.

*Phase Transitions in Tungsten Trioxide at Low Temperatures.* I. LEFKOWITZ, M. B. DOWELL, AND M. A. SHIELDS. Pitman-Dunn Laboratory, Frankfort Arsenal, Philadelphia, Pennsylvania 19137. Capacitance and electrical resistivity measurements have been made on stoichiometric and on oxygen-deficient tungsten trioxide crystals from 4.2 to 300°K. X-ray oscillation and rotation photographs were made on single crystals of both materials near 200°K and near 300°K. Capacitance and resistivity anomalies identify phase transitions near 40, 65, 130, 220, 260°K in stoichiometric WO<sub>3</sub>. Resistivity anomalies occur near 80, 130, 220 and 260°K in oxygen-deficient tungsten trioxide. Capacitance measurements suggest that the transformation at 130°K of a low-temperature phase to a high-temperature phase of stoichiometric WO<sub>3</sub> is associated with a doubling of the  $c$ -parameter of the unit cell. Resistivity measurements establish probable conduction mechanisms in each phase of stoichiometric and of oxygen-deficient tungsten trioxide, and show that oxygen-deficient tungsten trioxide undergoes a semiconductor-to-metal transition near 200°K. Electronic phenomena which do not appear to be associated with structural phase transformations are observed near 16°K in stoichiometric WO<sub>3</sub>.