

05.2-6 X-RAY STRUCTURAL STUDY OF LOW TEMPERATURE PHASE OF POTASSIUM CYANIDE. By Y. Yoshimura and K. Shimaoka, Department of Mathematics and Physics, Faculty of Science and Engineering, Ritsumeikan University, Tojiin-kitamachi, Kita-ku, Kyoto 603 Japan.

An as-grown crystal of potassium cyanide (KCN) undergoes two successive phase transitions at 168 (cubic-orthorhombic) and 83K (orthorhombic-orthorhombic), mainly involving orientations of the linear CN<sup>-</sup> ions in the crystal lattice (Suga, Matsuo & Seki, Bull. Soc. Jpn., 1959, 38, 1115-1124; Rowe, Rush & Prince, J. Chem. Phys., 1977, 66, 5147-5149). In addition to the above phase transitions, a phase which has been recognized widely as a metastable phase (space group Aa) exists in a small temperature region around 165K for a crystal subjected to repeated thermal cycles (Cimino, Parry & Ubbelohde, Proc. Roy. Soc., 1959, A252, 445-456; Parry, Acta Cryst., 1962, 15, 601-607). The crystal in this phase also undergoes a phase transition to an intermediate phase at 158K (Cimino et al., Proc. Roy. Soc., 1959, A252, 445-456). The purpose of this report is to describe the unit cells of the metastable phase of KCN crystal studied by X-ray method. Precession photographs showed multi-domain structures which were mutually related with a specific location of diffraction spots. The spots were able to be separated into several single domain patterns, and it was determined that the phase was the mixture of monoclinic and tetragonal patterns. Space group of the former lattice was uniquely determined to be A2/a with cell dimension a=8.28, b=4.58, c=7.61Å and β=109.2° at 163K. The data were different from Parry's (Acta Cryst., 1962, 15, 601) lattice parameters and space group which have been recognized widely. The latter has an incommensurate superstructure and its matrix lattice is constructed from [110], [110] and [001] directions of the cubic phase.

05.2-7 X-RAY AND OPTICAL STUDY OF FERRO-ELASTIC PHASE TRANSITION IN CsLiCrO<sub>4</sub> SINGLE CRYSTAL. By K.S. Aleksandrov, A.I. Kruglik, S.V. Melnikova, Institute of Physics, 660036 Krasnoyarsk, USSR

Among the crystals with general formula Me+LiBX<sub>4</sub> (Me+ = Rb, Cs, NH<sub>4</sub>; BX<sub>4</sub> = SO<sub>4</sub>, SeO<sub>4</sub>, BeF<sub>4</sub>, MoO<sub>4</sub>, WO<sub>4</sub>) there are known many ferroelectrics and ferroelastics.

The proper ferroelastic phase transition (PT) D<sub>2h</sub><sup>16</sup> → C<sub>2h</sub><sup>5</sup> at T<sub>0</sub> = 427 K was found recently in CsLiCrO<sub>4</sub> having the structure of β-tridimite type (Kruglik et al, Fizika Tverdogo Tela, 1986, 28, 1215-1217).

Optical and X-ray study of single crystals grown by Bridgman method were performed in temperature range 80-500 K. It was shown that birefringence changes, the optic indicatrix rotation in neighbour twin components, the temperature dependences of these values and of unit cell angle β(T) have the definite distinctions in respect to corresponding values for the isomorphous ferroelastic CsLiSO<sub>4</sub>. The nature of these distinctions is discussed on the basis of structural data.

05.2-8 FERROELECTRICS - SUPERIONICS. By V.K. Yanovskii and V.I. Voronkova, Department of Physics, Moscow State University, U.S.S.R.

Some oxide compounds are found to exhibit both ferroelectric properties and high ionic conductivity typical of superionic conductors, and may be considered as representatives of a new variety of solid state materials. They are TLNbWO<sub>6</sub> and RbNbWO<sub>6</sub> with the structure of defect pyrochlore type, Bi<sub>2</sub>WO<sub>6</sub> and a number of other bismuth-bearing compounds with layered perovskite-like structures, and the compounds of KTiOPO<sub>4</sub>-family. Single crystals of these compounds were grown from high-temperature solutions, and their crystallographic characteristics, domain patterns, dielectric and non-linear optical susceptibilities, electrical conductivity and other properties are studied. All the crystals proved to undergo structural transformations. In TLNbWO<sub>6</sub> and RbNbWO<sub>6</sub> these transformations take place in the range of 50 to 120°C and seem to be diffuse ferroelectric ones. The Bi<sub>2</sub>WO<sub>6</sub> undergoes a reconstructive transformation near 950°C between polar low-temperature orthorhombic phase and nonpolar high-temperature monoclinic phase, which can be classified as a pyroelectric phase transition. In Bi<sub>6</sub>Ti<sub>3</sub>WO<sub>18</sub> and Bi<sub>10</sub>Ti<sub>3</sub>W<sub>3</sub>O<sub>30</sub> the phase transitions are observed at 750 and 735°C, and are the first-order ferroelectric ones. In the crystals of KTiOPO<sub>4</sub>, RbTiOPO<sub>4</sub> and TlTiOPO<sub>4</sub> the second-order ferroelectric phase transitions take place at 934, 789 and 581°C.

The electrical conductivity of these compounds is mainly ionic and varies from 5·10<sup>-3</sup> to 10<sup>-6</sup> Ohm<sup>-1</sup>cm<sup>-1</sup> at 300°C with the activation energy of 0.1 to 0.3 eV. The conduction in Bi<sub>2</sub>WO<sub>6</sub> and related layered compounds results from fast migration of oxygen anions. In other crystals studied it is connected with the transfer of weakly bonded alkaline cations.

The presence of the mobile charged structural units appears to play an important role in the phenomena of electrical ordering. In addition, this can affect the formation of ferroelectric domains and lead to a strong low-frequency dielectric relaxation.