Structure and Jahn–Teller Effect in Mixed Crystals $Rb_2Cr_{1-x}Mn_xCl_4$—A Single Crystal Neutron Diffraction Study and Spectroscopic Results. G. MÜNNINGHOFF, W. TREUTMANN, E. HELLNER, G. HEGER, AND D. REINEN, Fachbereich Chemie der Philipps-Universitat, D-3550 Marburg 1, Germany. The structures of single crystals $\mathrm{Rb_2Cr_{1-x}Mn_xCl_4}$ ($0 \leq x \leq 1$) have been studied by neutron diffraction. A crystal of composition $x = 0.01$ shows a superstructure of the $\mathrm{K_2NiF_4}$ type [space group *Bbcm*; $a = b = 7.262$ Å, $c = 15.733$ Å]. The structural refinement [$R = 0.043$] yields an antiferrodistortive order of tetragonally elongated octahedra (superimposed by a small orthorhombic component) with Cr–Cl bond lengths of 2.43 Å ($\|[001]$) and 2.40 Å, 2.74 Å ($\perp[001]$). Structural results for $x = 0.01/0.08/0.53/0.63/0.83/0.91/0.97$ in space group $I4/mmm$[$\mathrm{K_2NiF_4}$Type]—in particular the anomalous *ms* displacements of Cl(1) in the (001) plane—give evidence that the distortion of the (Mn, Cr)$\mathrm{Cl_6}$ octahedra decreases with increasing x. AOM calculations based on experimental ligand field energies indicate that the individual $\mathrm{CrCl_6}$ polyhedra are more strongly distorted than the (Jahn–Teller stable) $\mathrm{MnCl_6}$ octahedra in mixed crystals with larger x values.

Stereochemical Active $(5s)^2$-Lone Pairs in the Structures of α-InCl and β-InCl. C. P. J. M. VAN DER VORST AND W. J. A. MAASKANT, Gorlaeus Laboratoires University of Leiden, P.O. Box 9502, 2300 RA Leiden, The Netherlands. The structures of both the yellow room-temperature (α) and the red high-temperature modification (β) of indium monochloride are interpreted in terms of the stereochemical active $(5s)^2$-lone pair of the monovalent indium ion. A local description is given, in which the pseudo-Jahn–Teller effect $(A_{1g} + T_{1u}) \times (t_{1u} + t_{2g})$ of the $\mathrm{InCl_6}$ octahedron plays the central role. There are three ways in which a free octahedron, with an $(ns)^2$ ion at the center may deform: tetragonal (a), digonal (b), and trigonal (c), in ascending order of stability. α-InCl consists of a rock salt-like packing of octahedra, roughly of the types b and c (ratio 3 : 5). β-InCl has the β-TlI structure, which may also be derived from a rock salt structure. The coordination polyhedron of the cation shows close relationship to the octahedron of type a. Comparison of the $\mathrm{InCl_6}$ and $\mathrm{ClIn_6}$ octahedra in α-InCl and calculation of the polarization energy of both α- and β-InCl show that the cation polarization is more important than the anion polarization.

A Kinetic Study of the System γ-AlOOH–Al_2O_3. S. J. WILSON AND J. D. C. MCCONNELL, Department of Mineralogy and Petrology, University of Cambridge, Cambridge, England. A time–temperature study has been made of the system γ-AlOOH (boehmite)–$\mathrm{Al_2O_3}$. The isothermal TTT diagram produced demonstrates the course of the transformation sequence, which involves a number of metastable transition alumina intermediate phases. This type of treatment allows calculation of kinetic parameters for the various transformation processes, and these may be correlated with the mechanisms operating. Kinetic aspects of variations in microstructure and crystal structure have also been studied. In particular, the progress of cation migration processes involved in the transformation γ- → δ-$\mathrm{Al_2O_3}$ has been followed in terms of the continuous variation of the spinel subcell parameters.

Shape Effects on Crystallite-Size Distributions in Synthetic Hematites from X-Ray Line-Profile Analysis. P. H. DUVIGNEAUD AND R. DERIE, Chef de Travaux, Service de Chimie Industrielle et de Chimie des Solides, Universite Libre de Bruxelles, Belgium. Synthetic acicular hematite shows a nonuniform broadening of the X-ray lines in a large temperature range. The factors affecting the peak broadening were studied by recording the powder line profiles of the (012), (014), (110), (024), and (116) reflections. The orientation relationships of these planes vs the main particle axes were previously checked by electron microdiffraction. On the other hand, various hematites having different particle sizes and shapes (spheres, slabs, needles) were investigated as well. The mean crystallite sizes were determined from a classical Fourier transform analysis whereas the size distributions were computed by a smoothing procedure described by Le Bail and Louër (19). The results show that the nonuniform broadening is ascribed to the shape anisotropy of the particles rather than to strains and faults broadening since (i) this last phenomenon is negligible in spherical-shaped particles, (ii) nonuniform broadening remains in acicular particles after further heating at 600°C, and (iii) a good estimate of the ratio of particle width to thickness has been found.

Electrical Ionic Conductivity and Optical Absorption Studies on Superionic Compound $RbAg_{4-x}Cu_xI_5$ Films. K. HARIHARAN, Department of Physics, Indian Institute of Technology, Madras—600 036, India. Electrical ionic conductivity studies on thin films of superionic compound $\mathrm{RbAg_{4-x}Cu_xI_5}$ ($x = 0$ to 0.4) have been carried out from 438 to 150°K. From the conductivity plots, the activation energy for $\mathrm{Ag^+}$ ion conduction has been calculated. Optical absorption studies on the above films indicate (i) the existence of silver colloids in the film, (ii) a forbidden internal transition in the free $\mathrm{Ag^+}$ ion becoming activated because of the structure of $\mathrm{RbAg_{4-x}Cu_xI_5}$, and (iii) a well-defined exciton state in the above material.