

Disorder and Ionic Polarons in Solid Electrolytes. W. J. PARDEE AND G. D. MAHAN. Physics Department, Indiana University, Bloomington, Indiana. The role of ion-ion repulsion and ion-phonon coupling in superionic conduction is explored. It is argued that the order-disorder phase transition is not associated with the conductivity discontinuity, but with a higher temperature second-order phase transition that has been seen in some super ionic conductors, and which we predict for others. The specific heat, ion distribution, and conductivity are calculated.

X ray and Neutron Diffraction Study of Intermediate Phases in Nonstoichiometric Cerium Dioxide. S. P. RAY AND A. S. NOWICK. Henry Krumb School of Mines, Columbia University, New York, New York 10027. AND D. E. COX, Physics Department, Brookhaven National Laboratory, Upton, New York 11973. Powder samples of reduced ceria $Ce_{2-x}O_{3-x}$ of known compositions in the range $0 < x < 0.3$ have been examined by X ray and neutron diffraction techniques to determine which intermediate phases belonging to the homologous series Ce_nO_{2n-2} (with $n = \text{integer}$) truly exist. Through the appearance of superlattice lines in the neutron diffraction patterns, the existence of four distinct phases, corresponding to $n = 7, 9, 10,$ and 11 was established. Aside from the phase Ce_7O_{12} , the structures of these phases cannot be accounted for with rhombohedral cells based on $\langle 111 \rangle$ vacancy strings, but indicate lower (monoclinic or triclinic) symmetry. The structure of Ce_9O_{16} and $Ce_{10}O_{18}$ do not agree with structures proposed for the analogous Pr_nO_{2n-2} compounds.

^{125}Te Mossbauer Spectra of the Te(IV) Oxides and Oxyfluorides. P. DOBUD AND C. H. W. JONES. Department of Chemistry, Simon Fraser University, Burnaby, B.C., Canada V5A 1S6. The ^{125}Te Mossbauer spectra of a number of Te(IV) oxides are reported in which the tellurium is present in either a distorted trigonal bipyramidal or distorted tetrahedral coordination with the lone-pair occupying one of the coordinate positions. The isomer shifts and quadrupole splittings are interpreted in terms of the relative s and p character of the stereochemically active lone-pair. Mossbauer data for $KTeF_5$, $K_2TeO_2F_2$, $Cs_2TeO_2F_2$, and Cs_2TeOF_4 are also presented and discussed.

Structural Studies in the Li_2MoO_4 - MoO_3 System. II. The High Temperature Form of Lithium Tetramolybdate, $H-Li_2Mo_4O_{13}$. B. M. GATEHOUSE AND B. K. MISKIN. Chemistry Department, Monash University, Clayton, Victoria, Australia, 3168. $H-Li_2Mo_4O_{13}$ crystallizes in the triclinic space group, $P\bar{1}$, with cell parameters $a = 8.612 \text{ \AA}$, $b = 11.562 \text{ \AA}$, $c = 8.213 \text{ \AA}$, $\alpha = 94.45^\circ$, $\beta = 96.38^\circ$, $\gamma = 111.24^\circ$, and $Z = 3$. The structure was solved using three-dimensional Patterson and Fourier techniques. Of the 4403 unique reflections collected by counter methods, 2883 with $I > 3\sigma(I)$ were used in the least-squares refinement of the model to a conventional R of 0.031 ($R_w = 0.035$). Like $L-Li_2Mo_4O_{13}$, $H-Li_2Mo_4O_{13}$ is a derivative structure of V_6O_{13} and can be related to $L-Li_2Mo_4O_{13}$ by movement of one of the shear planes in the structure.

Neutron Diffraction Determination of the Crystal Structure of Ce_7O_{12} . S. P. RAY. Henry Krumb School of Mines, Columbia University, New York, New York 10027. AND D. E. COX. Physics Department, Brookhaven National Laboratory, Upton, New York 11973. A neutron diffraction study has been made on polycrystalline and single-crystal samples of $Ce_{0.714}O_{1.714}$. The results confirm that the compound is isostructural with ternary oxides of the type UY_6O_{12} . The space group is $R\bar{3}$ with hexagonal unit cell dimensions $a = 10.37$ and $c = 9.67 \text{ \AA}$ (rhombohedral cell $a = 6.80 \text{ \AA}$ and $\alpha = 99.4^\circ$). The hexagonal unit cell contains three formula units of Ce_7O_{12} . Totals of 79 and 24 independent reflections from the single crystal were measured at neutron wavelengths of 1.185 \AA and 2.37 \AA , respectively. Simultaneous refinement of the two sets of data yielded a weighted R factor of 0.144. The structure is a rhombohedral defect type of fluorite arrangement in which pairs of oxygen vacancies are ordered along the $[111]$ axis.

Mechanism of the Solid State Synthesis of Cobalt Molybdate. JERZY HABER, ANNA SOSNOWSKA, AND JACEK ZIOLKOWSKI. Research Laboratories of Catalysis and Surface Chemistry, Polish Academy of Sciences, Krakow, Poland. Mechanism and kinetics of the solid state reaction $2CoO + 2MoO_3 + Mo = Co_2Mo_3O_8(1)$ was studied in the temperature range $500-1100^\circ C$ by chemical and X ray analysis. At three intergranular contacts existing in such powder mixture the following reactions proceed at comparable rates: $2MoO_3 + Mo = 3MoO_2(2)$, $MoO_3 + CoO = CoMoO_4(3)$,

and $8\text{CoO} + 3\text{Mo} = \text{Co}_2\text{Mo}_3\text{O}_8 + 6\text{Co}$ (4). Subsequent reactions of their products may be described by the equations: $3\text{Co} + 3\text{MoO}_3 = \text{Co}_2\text{Mo}_3\text{O}_8 + \text{CoO}$ (5), $2\text{CoO} + 3\text{MoO}_2 = \text{Co}_2\text{Mo}_3\text{O}_8$ (6), and $2\text{CoMoO}_4 + \text{Mo} = \text{Co}_2\text{Mo}_3\text{O}_8$ (7). Reaction (5) is very rapid, whereas (6) and (7) are slow. The path (4) + (5) is thus responsible for the first rapid step of (1), the subsequent slow step being due to (2) + (6) and (3) + (7). No metallic cobalt is found in products of (1) because of its very rapid consumption in (5): However, its role as intermediate was confirmed by magnetic measurements. Metallic cobalt is very reactive even at 300° with CoMoO_4 and MoO_3 . This hints to its important role in the reconstruction of the surface of cobalt molybdate catalysts in the course of the catalytic reaction.

The Crystal and Molecular Structure of bis(Ortho-Amino Benzoato) Copper (II), $\text{Cu}(\text{H}_2\text{NC}_6\text{H}_4\text{COO})_2$. BRUCE A. LANGE AND HELMUT M. HAENDLER. Department of Chemistry, University of New Hampshire, Durham, New Hampshire 03824. Bis(ortho-aminobenzoato) copper(II), $\text{Cu}(\text{H}_2\text{NC}_6\text{H}_4\text{COO})_2$, crystallizes in the monoclinic space group $P2_1/c$ with cell dimensions $a = 12.95(1)$, $b = 5.25(1)$, $c = 9.39(1)$ Å, and $\beta = 93.3(1)^\circ$. The structure was determined using three-dimensional X ray diffraction data gathered on multiple-film equi-inclination integrated Weissenberg photographs taken about two crystal axes. Refinement with anisotropic temperature factors led to $R = 3.1\%$. Coordination about the copper is that of a distorted octahedron. Four equatorial positions are occupied by two amino nitrogens and two carboxylate oxygens with both the nitrogens and oxygens in the trans positions. The octahedral coordination is completed in the axial positions by two carbonyl oxygens that do not originate from the same ligands that occupy the equatorial sites. Each copper in the (100) plane is attached to four other coppers via carboxylate bridges to give a two-dimensional polymeric network coincident with the (100) plane. Significant hydrogen bonding occurs to strengthen the two-dimensional network, which, it is suggested, accounts for the extreme insolubility and high thermal stability of the compound.