meters ($\underline{a}$ and $\underline{c}$) increase monotonically with increasing temperature but the $\underline{c}$ axis of the Mg^{2+}-Li^+ compound decreases rapidly between the temperature range $100°$-$220°C$ and starts to increase above $220°C$.

As yet there are not convincing proofs as to whether the anomaly in the thermal expansion should be attributed to phase transition as suggested by conductivity data or to a desorption of water from the interblock plane.

envisaged as associated in equal proportion in $H_5O_2^+$ and H_4O_2 dimers and this suggests a possible mechanism for proton conduction which can be probed by quasielastic neutron scattering.

For the single crystal neutron diffraction study of $Sr(Pr)Cl_{2.10}$ ($\lambda = 0.53$Å) it is demonstrated that the anion interstitials are of two types: ($\frac{1}{2}$vv) $v \approx 0.38$ and (xxx) x=0.285. The ratio of ($\frac{1}{2}$vv) interstitials to dopant cations is about 2.5. In contrast to the alkaline-earth fluorides, (www) $w \approx 0.42$ or 0.38 interstitials are not important in this system. Defect energy calculations on anion-excess strontium chloride suggests that the clusters proposed for the alkaline-earth fluorides are less important for $SrCl_2/MCl_3$. Clusters based on the aggregation of <111> cation substitutional/anion interstitial pairs provide a more favourable mode of defect cluster formation. A cluster model based on this type of aggregation provides a good model for our observed ratio of anion interstititals to dopant cations but does not explain the observed proportion of anion vacancies.

07.3-06   NEUTRON DIFFRACTION STUDIES ON FAST ION CONDUCTORS (I) DUO_2ASO_4 $4D_2O$ and (II) $Sr(Pr)Cl_{2.10}$. By P.J. Bendall[i], C.R.A. Catlow[ii], B. E. F. Fender[iii] and A. F. Wright[iii].

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Neutron diffraction studies are reported on two different types of fast ion conductor. In one, high resolution powder diffraction techniques are employed to detect hydrogen ordering effects and occupancies in the good proton conductor $DUO_2ASO_44D_2O$; in the other, a high resolution single crystal investigation has been used to accurately locate the chloride ion positions in the anion excess fluorite system $Sr(Pr)Cl_{2+x}$.

The isostructural layered hydrates $HUO_2PO_44H_2O$(HUP) and $HUO_2ASO_4.4H_2O$ (HUAS) display high proton conductivities near room temperature (A. T. Howe and M. G. Shilton, J. Solid State Chem. (1980), $\underline{34}$, 149). Profile analysis of $DUO_2ASO_44D_2O$ above the transition temperature of $290 \pm 3°K$ was carried out in the space group $P4/ncc$ with a = 7.160 and c = 17.634. The structure of DUAs is very similar to HUP, with planar networks of water molecules alternating with layers of $\{UO_2PO_4\}_n^{n-}$. The neutron diffraction study shows (i) only one of two crystallographically distinct sites in a square of water molecules is occupied by hydrogen atoms and the occupancy is 3/4; (ii) the hydrogen atoms directed towards the oxygen of an ASO_4^- group are linked to the oxygen of a water molecule; (iii) the remaining hydrogen atoms (8 out of 36) are associated with a single maximum in scattering density midway between two oxygen atoms of water molecules in neighbouring water layers. The water molecules can thus be

07.3-07   STRUCTURE INVESTIGATIONS IN FAST IONIC CONDUCTORS. By H. Schulz, MPI Festkörperforschung, 7 Stuttgart 80, Germany.

In fast ionic conductors one sort of ions may move rapidly through the crystal lattice. The densities of these ions are often distributed over large parts of the elementary cell. The smeared out densities are caused by shallow atomic potentials. These potentials are (at least in distinct directions) so flat, that already thermally activated ions may show large thermal vibrations or jump from their site into a neighbouring site.

The thermal vibrations of these ions may be analysed by so-called anharmonic temperature factors. The corresponding probability density maps can be calculated by the Fouriertransform of the anharmonic temperature factors. These pdf maps can then be used to determine the atomic potentials of the ions under consideration.

We have used these formalisms for the first time up to the sixth order. Furthermore, we could show that temperature factors based on the Gram-Charlier expansion work much more effective than those based on the Edgeworth expansion, which has been used earlier for this type of structure investigation of fast ionic conductors. These calculations were carried out with the program system Prometheus, which allows the refinements of anharmonic temperature factors based on the above mentioned formalisms.   (Zucker, Perenthaler, Kuhs, Bachmann, Schulz, J. Appl. Crystal., submitted)

We have determined such atomic potentials for several fast ionic conductors (e.g. Ag_3SI, Ag_2S, AgI, Li_3N, $LiAlSiO_4$). These potentials can then be used to measure the activation energy. Furthermore they give hints on phase transitions. For example the Ag-potential in α-Ag_3SI allows already to predict the phase transition to the low temperature γ-phase and to estimate the temperature of the phase transition.
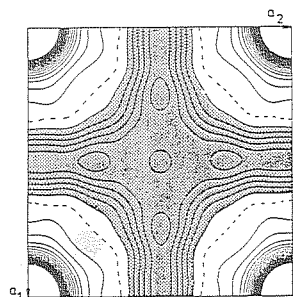
α-Ag_3SI (space group Im3m). Electron density at z=0. I atoms at the corners. Ag density is grey shadowed. Ag positions at (1/2,1/2,0) and (1/2,1/4,0)
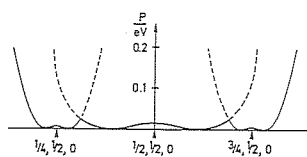
Ag potential in α-Ag_3SI. Black line: Potential for an Ag ion diffusing (1/4$\Leftrightarrow$3/4,1/2,0). Black and dotted line: Potential including Repulsion terms.

07.4-01 THE CRYSTAL STRUCTURE OF $Ru_6Cu_2C(CO)_{16}(MeCN)_2$.
Gerald B. Ansell, M. E. Leonowicz and Michelle A. Modrick, Analytical and Information Department and J. S. Bradley, Corporate Research Laboratories, Exxon Research and Engineering Company, P. O. Box 45, Linden, NJ 07036.

The title compound is one of several ruthenium/copper carbonyl clusters which have been synthesized as models of potential catalysts for reactions between carbon monoxide and hydrogen. The cluster was synthesized by reacting $Ru_6C(CO)_{16}^{2-}$ with $Cu(CH_3CN)_4^{+}$ in acetone. Single crystals were grown from methylene chloride/hexane solution and for diffraction purposes were sealed in a capillary tube with mother liquor. The crystals are triclinic with cell-dimensions a = 10.122(2), b = 16.364(2), c = 9.874(2) Å, α = 97.35(1), β = 96.58(2), γ = 77.89(1)° and have a space-group P$\bar{1}$. The structure was solved by direct methods and 6215 independent reflections have been refined to an R value of 0.059. The structure has a unique eight metal-atom cluster containing an almost regular octahedron of six ruthenium atoms. One copper atom is situated almost at the center of one of the triangular faces of the octahedron and the second almost over the center of one of the sides of the same triangle, 2.68Å from the first copper atom. A carbido carbon is found at the center of the Ru_6 cluster. Metal-metal bond distances are 2.80-3.07 Å for Ru-Ru, 2.55-2.81 for Ru-Cu. There are 13 terminal and 3 bridged carbonyls linked to Ru_6 octahedra. Each copper atom retains one acetonitrile ligand.

07.5-01 STRUCTURAL ORDERING IN $TbFe_2$ AND YFe_2.
By P. D'Antonio and J. H. Konnert, Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, D. C. 20375, and J. J. Rhyne and C. Hubbard, National Bureau of Standards, Washington, D. C. 20234.

Experimental radial distribution functions (RDF) for sputtered amorphous rare earth-transition metal compounds of YFe_2 and $TbFe_2$ have been determined. Errors due to an incorrect background, scaling of the data and termination effects have been minimized. Total neutron diffraction data were analyzed for YFe_2, whereas both total neutron and x-ray diffraction data were used for $TbFe_2$ in order to verify peak assignments in the RDF curves. The coordination numbers, internuclear distances and disorder parameters for the first six coordination spheres have been determined using the RADILS program (P. D'Antonio and J. H. Konnert, J. Appl. Cryst. (1979), 12, 634-635). The bonding topology in these materials is different than that found in their crystalline Laves phase structures. The radial distribution function, rG(r), corresponding to the topology in crystalline YFe_2-C is shown at the top of the figure. The transition metal substructure consisting of corner sharing tetrahedra is preserved in the metallic glass but the tetrahedral coordination of the rare earth atoms is not. The experimental rG(r) functions corresponding to the raw unsmoothed neutron data for YFe_2-R, the smoothed neutron data for YFe_2-N and $TbFe_2$-N and the smoothed x-ray data for $TbFe_2$-X are illustrated in the figure. The data were smoothed with a new variable filter digital FFT smoothing routine. The bulk density, ρ_o, and error estimates based on random errors in the unsmoothed, σ, and smoothed, σ_s, intensities are also shown.