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PS-10.01.10 X-RAY DIFFRACTION STUDY OF Nd_2CuO_4 By I.P. Makarova*, V.N. Molchanov, R.A. Tamazyan and V.I. Simonov, Institute of Crystallography, Russian Academy of Sciences, Moscow, Russia; M. Blomberg and M. Merisalo, Department of Physics, University of Helsinki, Helsinki, Finland.

Single-crystal X-ray diffraction studies have been carried out on Nd_2CuO_4, a parent structure for electron-doped superconductors, at 296K and 20K. The data have been collected on a spherical specimen (0.0140(5) cm in diam.), previously tested for absence of violations of the space group I4/mmm, and for absence of twinning.

In the specimen under study, the refined site occupancies indicate deficiency in neodymium (q_{Nd}=0.945(1)) and oxygen content (q_{O1}=0.922(1)). The results of our investigation show the significant deviation of the displacement parameters of Nd from the harmonic law. From the obtained structure parameters, the deformation electron density distribution has been determined. This distribution shows the peak of 4f electrons and an asphericity of the inner shells of electrons for the Nd atom. The residual density peaks of 3d electrons of the Cu atom are also observed. Recent results from this study will be presented and discussed.

PS-10.01.11 ON THE STRUCTURE OF SUPERCONDUCTING ORTHO-II PHASE OF $YBa_2CU_3O_{6.51(5)}$. By Thomas Zeiske, Dietmar Hohlwein and Rainer Sonntag, Hahn-Meitner-Institut Berlin and Institut für Kristallographie der Universität Tübingen, D-1000 Berlin 39, Glienicker Str. 100, Germany.

Our studies of oxygen ordering in superconducting $YBa_2Cu_3O_{6.51(5)}$ (Tc=56K) by single crystal X-ray diffraction lead to a quantitative structure for the ortho-II phase in the Y-Ba-Cu-O system.
From the intensities of superstructure reflections, we derived a structural model that confirms the ortho-II type of oxygen ordering by alternation of Cu-O-Cu and Cu-Cu chains in the basal plane. Furthermore, and probably most important, we could show that the asymmetric oxygen coordination of Ba cations caused by this oxygen ordering leads to displacements of Ba. The Ba cations shift by about 0.034Å in the [100] direction towards the Cu-O-Cu chains (Zeiske et al.(1992). Physica C, **194**,1).
These displacements are confirmed by anomalous scattering near the K absorption edge of Ba observed by synchrotron X-ray diffraction. Changes in structure factors of (h/2 0 0) ortho-II superstructure reflections are due to Ba displacements. Possible contributions from displacements of other atoms were found to be 5(13)% of barium contribution (Zeiske et al. (1993). Physica C, in press). A rigid ion model shows that the Ba displacements stabilize the ortho-II structure by reducing its lattice energy. The Ba shift calculated by the model for δ = 0.039Å is in close quantitative agreement with the experimental observations.

PS-10.01.12 NEW SUPERSTRUCTURE IN $YBa_2Cu_3O_{6.6}$ DETERMINED BY X-RAY DIFFRACTION. By R. Sonntag*, D. Hohlwein and Th. Zeiske, Institute of Crystallography, University of Tübingen and Hahn-Meitner-Institut, Berlin, Germany.

The superconducting transition temperature, T_c, of the high temperature superconductor $YBa_2Cu_3O_{6+x}$ is known to depend not only on the oxygen stoichiometry, but also on the specific ordering of the oxygen atoms in the basal Cu-O planes. Such details are established by precise structure determinations, which can only be performed by neutron or X-ray diffraction.

We succeeded in the determination of two different oxygen superstructures with x=0.35 (Sonntag et al. (1991). *Phys. Rev. Lett.*, **66**, 1497; Zeiske et al. (1992a). *Z. Physik* **B86**, 11) and with x around 0.5, for the so-called Ortho-II phase (Zeiske et al. (1991). *Nature* **353**, 542; Zeiske et al. (1992b). *Physica* **C194**, 1).

X-ray measurements on a $YBa_2Cu_3O_{6.6}$ crystal have shown a new superstructure with wave vector (0.55, 0, 0). We found 8 symmetry independent superstructure reflections in the hk0 layer. Q-scans over the superstructure reflections in the directions of the reciprocal axes did not show broadening with respect to Bragg reflections. A detailed structure determination is in progress and will be presented at the conference.

PS-10.01.13 CRYSTALLINE AND MAGNETIC ORDERING IN THE MONOCLINIC PHASE OF THE LAYERED PEROVSKITE PAMC. By P. Harris*, B. Lebech, Department of Solid State Physics, Risø National Laboratory, Denmark, F.K. Larsen, Department of Chemistry, University of Århus, Denmark, and N. Achiwa, Department of Physics, Kyushu University, Japan.

The layered perovskite $(CH_3CH_2CH_2NH_3)_2MnCl_6$ (PAMC) is an example of an antiferromagnet that shows weak ferromagnetism. The small ferromagnetic moment is believed to originate in anisotropic exchange interactions of the form $\mathbf{D} \cdot (\mathbf{S_1} \times \mathbf{S_2})$ (N. Achiwa, T. Matsuyama and T. Yoshinari, Phase Transitions 1990, **28**, 79.), an interaction which is possible because the low crystal symmetry allows the magnetic moments in the pure antiferromagnet to tilt without change of symmetry. In addition PAMC exhibits a large sequence of structural phases. It consists of $(MnCl_6)$ octahedra sandwiched between propylammonium chains. The ammonium group hydrogens may bond to the Cl^- ions in the octahedra in four different positions (P. Muralt, R. Kind and W. Bührer, Phys. Rev. B, 1988, **38**, 666.). At high temperatures all four positions are equally possible (tetragonal symmetry), but upon cooling there is a gradual freezing of the bonds and the structure becomes orthorhombic and finally monoclinic.
In order to understand the interactions between the crystal structure and the magnetic structure we have performed an elastic neutron scattering experiment and a 4-circle X-ray experiment on the low temperature monoclinic ξ phase of PAMC. The neutron experiment was done on the double axis spectrometer TAS3 at DR3, Risø, Denmark, using neutrons of wavelength 1.29 Å. The X-ray experiment at 8 K was done at Department of Chemistry, University of Århus, Denmark, using MoK_α radiation.
We have determined the crystal structure of the low temperature ξ phase in superspace group $P^{P2_1/c}_{1s}$ with a modulation vector of $\frac{1}{3}\mathbf{c}^*$. In addition, the temperature dependence has been determined of the monoclinic distortion and of the intensities of the satellite reflections. So far our conclusion is, that there seem to be strong interactions between the magnetic structure, the monoclinic distortion and the modulation wave.

