characterized by an ordered arrangement of short and long Nb-O-bonds.
In order to verify the results of the computational modeling, single crystal X-ray diffraction measurements have been carried out using synchroton radiation at Hasylab beamline F1. The diffraction data between 200K and 98K are refined on the basis of the calculated Ima2-structure. The ferroelectric order parameter as a function of temperature is obtained and the contributions of various distortional modes are assessed.
While the ab-initio structure calculations imply a purely displacive mechanism of the ferroelectric phase transitions in CNO, anisotropic diffuse scattering intensity that is observed in the X-ray diffraction data indicates local deviations from cubic symmetry in the paraelectric phase. The deviations correlate along <110>, giving rise to sheets of diffuse scattering normal to these directions [3]. In order to investigate the possible order-disorder contributions to the ferroelectric phase transitions, Monte Carlo simulations of a modified 12-state Potts-model on a pyrochlore lattice have been conducted. The equilibrated spin configurations of the model serve to generate supercells of CNO with local Nb-offsets from the center of their coordination polyhedra. The calculated diffraction image based on these supercells reproduces the measured diffuse scattering data qualitatively correct.

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Crystal Structure Analysis of Some Metallic Pyrochlores. Yoshitaka Matsushita[a], Kenya Ohgushi[b], Yoshio Katsuya[c], Masahiko Tanaka[a]. [a]*NIMS-Spring8,NIMS, Japan.* [b]*ISSP ,the University of Tokyo, Japan.* [c]*SPring-8 Service Co., Japan.*
E-mail: Matsushita.Yoshitaka@nims.go.jp

Recent years, the pyrochlore-type compounds ($A_2B_2X_7$ or $A_2B_2X_6$) are very interesting in the field of solid-state physics. For example, $Cd_2Re_2O_7$ [1] and AOs_2O_6 (A = K, Rb, Cs) [2] show superconducting properties and $Cd_2Nb_2O_7$ shows ferroelectric. Most of the properties may be strongly correlated with the structure. The pyrochlore structure has infinite three-dimensional substructure of B-X octahedrons. If we pointed out only B element, the B element forms infinite three-dimensional subunit of B…B tetrahedrons so called as pyrochlore lattice in physics field. This pyrochlore lattice is an origin of strong geometrical frustration effect, and the effect may give a driving force to generate the specific properties such as superconductivity, GMR ($Tl_2Mn_2O_7$) [3], and M-I transition ($Cd_2Os_2O_7$) [4]. On the other hand, as a result of recent study, under low temperature many of pyrochlore-type compounds clearly showed the consecutive structural phase transition with breaking inversion symmetry like the perovskite-type ferroelectric compounds, and the origin of ferroelectrics of the pyrochlore compounds is still unclear. In this study, we are focused on lead-heavy transition metal pyrochores ($Pb_2Ru_2O_7$ and $Pb_2Ir_2O_7$) which have show metallic behavior, and their structural details are also unknown. Therefore, we report the crystal structural details of the compounds ($Pb_2Ru_2O_7$ and $Pb_2Ir_2O_7$). The samples are successfully synthesized by a solid-state reaction. Intensities are measured by powder-diffraction method using high-resolution synchrotron radiation (Spring-8, Japan) at room temperature. Crystal structures are refined by Rietveld method with RIETAN-FP. Both of compounds show the acentric pyrochlore structure with F-43m. The crystallographic details will be presented.

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Neutron Diffraction Studies of New Magnetoelectric Perovskites. R. Tellgren[b], S.A. Ivanov[a,b], P. Nordblad[c], C. Ritter[d]. [a]*Dept of Inorganic Materials, Karpov' Institute of Physical Chemistry, Moscow, Russia.* [b]*Dept of Materials Chemistry, The Angstrom Laboratory, Uppsala University, Sweden.* [c]*Dept of Engineering Sciences, Uppsala University, Sweden.* [d]*Institut Laue-Langevin, Grenoble Cedex, France.*
E-mail: rte@mkem.uu.se

Magnetoelectrics are materials that are both ferroelectric and ferromagnetic in the same phase. These compounds have potential applications in a whole range of new functional materials. Perovskite oxides containing Pb and Bi cations are particularly promising candidates. Current neutron powder diffraction studies at ILL were focused exclusively on some new and less well studied, but potentially interesting magnetoelectric perovskites.
Pure powder samples were prepared by ceramic technology. X-ray analysis indicated that the compounds have a perovskite-related structure. Magnetic and dielectric measurements were made between 1.5-700 K in order to obtain information about the coexistence range of magnetic and ferroelectric properties. Detailed neutron powder diffraction (NPD) investigations were performed in the temperature range 10-700 K using the D1A diffractometer (ILL, Grenoble, France). NPD powder patterns were registered in the two-theta range 10-160° using λ=1.91 A. The Rietveld method was used for the refinement of the nuclear and magnetic structures.