

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 synchrotron 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  $\langle 110 \rangle$ , 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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**Keywords:** ferroelectrics; diffuse scattering; pyrochlore

#### FA2-MS05-P11

**Crystal Structure Analysis of Some Metallic Pyrochlores.** Yoshitaka Matsushita<sup>a</sup>, Kenya Ohgushi<sup>b</sup>, Yoshio Katsuya<sup>c</sup>, Masahiko Tanaka<sup>a</sup>. <sup>a</sup>NIMS-Spring8, NIMS, Japan. <sup>b</sup>ISSP, the University of Tokyo, Japan. <sup>c</sup>Spring-8 Service Co., Japan. E-mail: [Matsushita.Yoshitaka@nims.go.jp](mailto: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 pyrochlores ( $Pb_2Ru_2O_7$  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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#### FA2-MS05-P12

**Neutron Diffraction Studies of New Magnetoelectric Perovskites.** R. Tellgren<sup>b</sup>, S.A. Ivanov<sup>a,b</sup>, P. Nordblad<sup>c</sup>, C. Ritter<sup>d</sup>. <sup>a</sup>Dept of Inorganic Materials, Karpov' Institute of Physical Chemistry, Moscow, Russia. <sup>b</sup>Dept of Materials Chemistry, The Angstrom Laboratory, Uppsala University, Sweden. <sup>c</sup>Dept of Engineering Sciences, Uppsala University, Sweden. <sup>d</sup>Institut Laue-Langevin, Grenoble Cedex, France.

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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  $\lambda=1.91$  Å. The Rietveld method was used for the refinement of the nuclear and magnetic structures.

**$\text{Bi}_{0.5}\text{Pb}_{0.5}\text{Fe}_{0.5}\text{Zr}_{0.5}\text{O}_3$** 

This compound crystallizes in orthorhombic space group  $Pb_{21}m$  with  $a \approx \sqrt{2}a_p$ ,  $b \approx 2\sqrt{2}a_p$  and  $c \approx 2a_p$  (with  $a_p \approx 4.04$  Å), and exhibits antiferromagnetic order below 450 K. The refinement of the magnetic structure at 10 K shows that the  $\text{Fe}^{+3}$  ions order with a propagation vector  $k = (0,0,0)$  and a magnetic moment of  $4.1(1) \mu_B$ .

 **$\text{Ba}_2\text{CoTeO}_6$** 

It was found that at 295K the perovskite crystal structure is trigonal, space group  $P-3m$ , and contains a completely ordered array of the  $\text{CoO}_6$  and  $\text{TeO}_6$  octahedra. When the temperature is decreased, this compound undergoes an AFM phase transition below 20K and magnetic diffraction peaks were observed. These new peaks are forbidden for crystallographic Bragg reflections in the space group  $P-3m$ . The antiferromagnetic structure at 10K was characterized by a propagation vector of  $k = (1/2, 1/2, 0)$ ; this structure shows an ordered magnetic moment of  $2.4(1) \mu_B$  for the  $\text{Co}^{2+}$  ions.

 **$\text{Pb}_2\text{CoTeO}_6$** 

At room temperature this complex perovskite can be described as a hexagonally distorted perovskite structure ( $a=5.676(1)$ ,  $c=13.852(1)$  Å *s.g.*  $P6_3/mmc$ ). Above the ferroelectric phase transition ( $T_c=380\text{K}$ ) the structure was found as a cubic ( $a=8.032(1)$  Å, *s.g.*  $Fm-3m$ )

Below the antiferroelectric phase transition at 200K the best fit was obtained for a monoclinic structure (space group  $P2_1/n$ ,  $a=5.663(1)$ ,  $b=5.680(1)$ ,  $c=8.019(1)$  Å,  $\beta=90.19(1)^\circ$  and considering a site disorder of cations Co/Te. With decreasing temperature this compound undergoes an antiferromagnetic phase transition phase near 25K and several magnetic reflections were registered. The antiferromagnetic structure at 5K was characterized by a propagation vector of  $k = (1/2, 0, 1/2)$  and an ordered magnetic moment of  $2.5(3) \mu_B$  for the  $\text{Co}^{2+}$  cations.

**Keywords: magnetoelectric; neutrons; perovskite**

**FA2-MS05-P13****Synthesis of a New Compound Based on Tin (II) with Intermediate  $\text{SnX}_4\text{E}$  and  $\text{SnX}_5\text{E}$  Geometry.**

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Hybrid compounds based on tin (II) are very rare, i.e. there are only two structures reported in literature with a general formula hydrazinium(2+) [trifluorostannate(II)] [3]. Recently, two other structures including  $\text{SnF}_3^-$  has been synthesized and structurally determined [1], [2]. This work deals with the first hybrid of tin (II) where tin atom take up the  $\text{SnX}_4\text{E}$  geometry. The crystal structure of  $\text{C}_{12}\text{H}_{14}\text{N}_2^{2+}$ ,  $(\text{Sn}_2\text{F}_6)^{2-}$  was determined using X-ray single-crystal diffraction. Characterizations with Mössbauer spectroscopy and electric conductivity will be given. The title compound is built up  $\text{SnF}_3^-$  anions and 1,1'-biphenyl-4,4'-diamonium, diprotonated organic ring. hydrogen bonds of N-H...F and N-H...O ensure the cohesion of the hydride structure .

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