distribution maps obtained from the maximum entropy method (MEM) describe that 13.4 % of protons exist at inter-layer space. Proton diffusion constants were estimated as $1.9(1) \times 10^{-10}$ $m^2/s$ at 393 K and $2.1(3) \times 10^{-10}$ $m^2/s$ at 413 K respectively. The structural change corresponds to a rotational mode of $SeO_4$ tetrahedra, which is led from the group theoretical analysis from *R3m* to *C2/c*. A diffusive spectrum was observed around 0 meV at the L-point (0.5 2 0) above $T_C$ as an over dumped phonon mode. The rotational mode of $SeO_4$ tetrahedra drives the improper ferroelastic phase transition, and assists the disconnection and reconstruction of hydrogen bonds in the high temperature phase.

Keywords: neutron diffraction elastic and inelastic, proton conductivity, phase transitions

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### X-ray diffuse scattering and a local structure of $(CH_3)_4NCdCl_3$ (TMCC) and related compounds

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A local structure of TMCC has been determined by configurational-bias reverse Monte Carlo method basing on X-ray diffuse scattering data. Two phases have been analysed and refined: phase I at 293 K, $P6_3/m$ space group, $a$ = 0.9139(1) nm, $c$ = 0.6723(1) nm, and phase I' at 410 K, $P6_3/mmc$ space group, $a$ = 0.9235(1) nm, $c$ = 0.6742(1) nm. A model dividing $CdCl_6$ octahedra chains into elementary bricks has been implemented in order to take into account coupling between orientation of TMA molecules and local deformations of the octahedra chains. The resulting structures contain the subchains of $CdCl_6$ octahedra shifted longitudinally away from their average positions. Their lengths show the Poisson-like distribution with an average value of about 6 unit cells. X-ray diffuse scattering effects observed on the *hk*0 plane require the existence of the transverse subchain displacements. Additional transversal correlation between longitudinal shifts of the subchains is needed to explain weak modulation effects and diffuse streaks observed on the planes perpendicular to ***c****.

Keywords: disordered systems, diffuse scattering, reverse Monte Carlo

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### Magnetoelastic effects in $BiMn_2O_5$: A high-resolution synchrotron x-ray diffraction study

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Multiferroic materials with coexisting (anti)ferromagnetism and ferroelectricity have attracted renewed attention, due to the interesting physics involved as well as relevant potential applications in spintronics. A fairly strong coupling amongst ferroelectric and magnetic order parameters may occur as a result of exchange striction effects in magnetic structures lacking an inversion center. Below the magnetic ordering temperature, slight atomic displacements take place and strengthen (weaken) the satisfied (frustrated) interactions, breaking the inversion symmetry of the structure and leading to ferroelectricity. In this work, synchrotron x-ray diffraction measurements were performed on single crystalline and powder samples of $BiMn_2O_5$. A linear temperature dependence of the unit cell volume was found between TN=38 K and 100 K, suggesting that a low-energy lattice excitation may be responsible for the lattice expansion in this temperature range. Between T* ~65 K and TN, all lattice parameters showed incipient magnetoelastic effects, due to short-range spin correlations. An anisotropic strain along the a-direction was also observed below T*. Below TN, a relatively large contraction of the a-parameter following the square of the average sublattice magnetization of Mn was found, indicating that a second-order spin Hamiltonian accounts for the magnetic interactions along this direction. Polycrystalline samples grown by distinct routes and with nearly homogeneous crystal structure above TN presented structural phase coexistence below TN, indicating a close competition amongst distinct magnetostructural states in this compound.

Keywords: $BiMn_2O_5$, multiferroics, high-resolution x-ray powder diffraction

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### A strategy to prepare multiferroic materials

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Manganese doped bismuth titanate is a potential multiferroic material, displaying both ferroelectricity and ferromagnetism. This is because of the layered nature of the Aurivillius structure which involves the stacking of octahedral perovskite blocks in between layers of bismuth oxide. An n=3 Aurivillius structure, with 3 layers of octahedral units in the perovskite block, are of special interest to solid state chemists. This is because the n=3 arrangement, provides simultaneously, a locally symmetric environment for the B-cations in the middle octahedral layer of the perovskite block and also a structurally distorted environment for the B-cations in the top and bottom octahedral layers of the perovskite block. The stability in maintaining this structural distortion is due to the 6s2 lone pair of electrons from the bismuth in the bismuth oxide layer. This unique structure can accommodate the usually conflicting requirements of ferroelectric and ferromagnetic properties to coexist. The objective would be to incorporate a layer of magnetic manganese cations within the middle octahedral layer, which benefits from the symmetrical environment, and integrate titanium into the top and bottom octahedral layers. This would introduce ferromagnetic properties to bismuth titanate, which is already a well-known ferroelectric material. Synchrotron X-ray diffraction has already been used to determine the structure of some of these compounds and together with magnetic property measurements, it is a step forward in uncovering the relationship between the observed ferroelectric and ferromagnetic properties of these compounds and their atomic structure.

Keywords: materials structure and characterisation, X-ray