that the large structural changes are accompanied with the successive phase transitions.

Keywords: inorganic organic compounds, neutron X-ray scattering, structural phase transitions

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**Powder neutron diffraction studies of inorganic ferroelectric phase transitions**

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We shall present some of our recent results on the nature of the ferroelectric-paraelectric and other phase transitions in a variety of inorganic systems, as studied by variable temperature powder neutron diffraction. Examples will include the contrasting behaviours of the Aurivillius family of layered perovskites including SrBi2Ta2O9 and Bi2WO6; the former involves simply ‘octahedral tilt’ type transitions, whereas the latter involves a reconstructive transition from corner-shared to edge-shared octahedra. Other examples will include the unusual layered oxyfluoride Na3WO4F3, which exhibits a remarkably high TC for a fluoride (~ 800K), and which shows 3 ferroelectric phases below TC. Finally, the important multiferroic BiFeO3 has been studied, and we will comment on its structural behaviour versus temperature, especially around TC, and including the possibility of a cubic paraelectric phase.

Keywords: ferroelectric, powder neutron diffraction, phase transitions

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**Structural phase transitions in trans-1,2-diaminocyclohexane derivative**

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trans-1,2-Diaminocyclohexane, a rigid molecule of C2 symmetry and two equatorial C-N bonds, was used as a chiral element of hydrogen-bonded networks and also as a bidentate ligand for chiral catalysts. We reported the synthesis and room temperature crystal structure of trans-(1R,2R)-N-acetyl-N’,N”-di-(4-bromophenyl)-1,2-diamino cyclohexane [1]. Quite unexpectedly we have found out two reversible phase transitions in the temperature range 100-295K. The previously published room-temperature crystal structure is monoclinic P21, with Z=1. The structure is disordered: one of the bromine atoms occupies two alternative positions with equal probability (s.o.f.’s are 0.5). The anisotropic refinement of bromine atoms in both positions was very stable and led to perfectly reasonable geometries and Uij values. On cooling down, below ca. 250K, the crystal undergoes the continuous phase transition to another monoclinic P21 phase, with a doubled value of the c unit-cell parameter, and two symmetry-independent molecules (Z’=2). The attempts were made to refine either the room temperature structure in the low temperature unit cell or vice versa, but none of these refinements led to reasonable results. Of course room temperature structure could be refined in a bigger unit cell, but the final effect was inferior to the original one. Above all, the new refinement did not lead to the ordering of bromine atoms, and some displacement parameters became non-positive determined. Below 160K another phase transition takes place, this time to the triclinic P1 space group with two molecules in the unit cell (i.e., Z’=2). Both phase transitions are reversible; we were able to use the same crystal many times and observe the same diffraction patterns.


Keywords: phase transitions, intermolecular interactions, disorder

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**Order parameters for phase transitions to structures with incommensurate modulations**

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Given the k vector for a distortion in a parent crystalline structure, what resulting space-group symmetries are possible? We have answered this question (Stokes, Campbell & Hatch, 2007, Acta Cryst. A63, 365) for the case of one-dimensional incommensurate modulations where the resulting symmetries are described by (3+1)-dimensional superspace groups. Most recently, we have extended our group theoretical methods to the general case of any arbitrary set of N modulations where the symmetries are described by (3+N)-dimensional superspace groups.

Keywords: phase transitions in solids, incommensurate modulated structures, group theory

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**Spontaneous strain in superconductors**

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Recently, the change in the orthorhombicity of the high-temperature superconductor YBa2Cu3O6.5 at the superconducting transition temperature Tc could be clearly detected by accurate lattice parameter measurement [1]. The introduction of a new critical exponent was considered necessary for explaining the result. The very small anomaly of the lattice parameters of intermetallic superconductor MgB2 was also clearly observed near Tc [2]. This anomaly was considered to be independent of the superconductivity onset. We could also clearly detect the change in the lattice parameter of the high-temperature superconductor La1.85Sr0.15CuO4 at Tc. [3]. For the first time, we showed that the change can be attributed to a spontaneous strain in the superconducting phase caused by the coupling between a superconducting order parameter and the strain. We indicated that the anomaly in MgB2 can also be understood on the basis of the same coupling. Similar experiments on conventional superconductors are necessary to clarify whether such a phenomenon is common to all superconductors. We carried out powder X-ray diffraction experiments on Ba0.8K0.2B6O13, which is a well-studied conventional superconductor with a simple cubic perovskite structure. The diffraction patterns were analyzed by the Rietveld