

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 $\text{SrBi}_2\text{Ta}_2\text{O}_9$ and Bi_2WO_6 ; 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 $\text{Na}_5\text{W}_3\text{O}_9\text{F}_5$, which exhibits a remarkably high TC for a fluoride ($\sim 800\text{K}$), and which shows 3 ferroelectric phases below TC. Finally, the important multiferroic BiFeO_3 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 C_2 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*-(1*R*,2*R*)-*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 $P2_1$, 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 U_{ij} values. On cooling down, below ca. 250K, the crystal undergoes the continuous phase transition to another monoclinic $P2_1$ 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.

[1] M.Kwit et al., *Pol.J.Chem.* 77 (2003) 1669.

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 $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ at the superconducting transition temperature T_c 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 MgB_2 was also clearly observed near T_c [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 $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ at T_c [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 MgB_2 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 $\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_3$, which is a well-studied conventional superconductor with a simple cubic perovskite structure. The diffraction patterns were analyzed by the Rietveld