method to obtain accurate lattice parameters. The Meissner effect was also measured to determine the T_c. The change in the lattice parameter of $Ba_{0.6}K_{0.4}BiO_3$ could be detected at T_c, which can be attributed to the spontaneous strain in the superconducting phase. We can conclude that this phenomenon is common to all superconductors.
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Charge ordering, isosymmetrical phase transitions and magnetic properties of mixed valence vanadates

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The mixed valence vanadates $MV^{3+}V_3^{4+}O_8$ (M=Yb, Y, Lu) are structurally related to $CaFe_2O_4$ and are build of a framework of VO_6-octahedra [1,2]. Two different phases (α and β), which differ only in the arrangement of the trivalent M-cations, are known. Their similarity favours the occurrence of polytypism. The magnetic susceptibility shows anomalies for the β-phases at ≈185 K (YbV_4O_8, [3]) and 190 K (YV_4O_8, [2]), respectively. For the α-phases, the anomalies occur below 100 K. Powder and single crystal diffraction as well as specific heat studies confirm the existance of first order isosymmetrical structural phase transitions. While above the phase transition the bond valence sums indicate no clear charge separation of the tri- and tetravalent V-ions, below the transition temperature a complete charge ordering is observed. The magnetic transitions can be understood assuming that the Curie-Weiss type d-electrons of the vanadium cations in the high temperature phases separate at the phase transition into d-electrons, which maintain their Curie-Weiss character and others, which lose their spin moment. The unusual complete charge ordering can thus be attributed not only to Coulomb repulsion between the cations, but also to possible spin gap formation [3]. Lattice parameter of the α-phase show a clear domain size effect: for samples with large domain sizes (≥ 100 Å) they show a smooth behaviour down to the phase transition temperature (65 K), while for samples with small domain sizes (≤ 40 Å) they are influenced by the phase transition in the β-phase (180 K).
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Keywords: isosymmetrical phase transition, charge order, composit crystal

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Neutron diffraction study of quantum effects on structural phase transition in quartz

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A phenomenological theory describes the temperature dependences of the order parameter Q, which is atomic shifts in displacive structural phase transition, and of strain e, which is coupled to Q, near a phase transition. We can describe their temperature dependences at low temperature if we use the quantum expansion of a potential [1]. We carried out the X-ray structure analysis of quartz, which shows a structural phase transition at approximately 850K, at various temperatures between 298 and 1126K using a single crystal [2]. The atomic shift of Si and the change in the strain were shown to obey the classical phenomenological theory. Recently, Romero and Salje have carried out a precise X-ray lattice parameter measurement of quartz in the temperature range of 30-300K [3]. They showed that the strain obeys the quantum phenomenological theory with a characteristic temperature of 187K. Direct evaluation of the quantum phenomenological theory by measuring the order parameter in the entire temperature range is required to verify the effectiveness of the theory. We carried out the structure analysis of quartz by powder neutron diffraction at several temperatures in the temperature range of 10-250K. Powder neutron diffraction patterns were obtained using a high-resolution powder diffractometer with 64 detectors. The diffraction patterns were analyzed by the Rietveld method. Squares of the shift of the Si atom along the a-direction and the strain were found to show the proportional dependence of each other in the entire temperature region. The effectiveness of the theory was directly verified by the atomic shift.
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Effect of temperature and pressure on the crystal structure of NaV_6O_{11}

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Since the discovery of its anomalous resistivity and ferrimagnetism, NaV_6O_{11} received wide interest. Its structure ($P6_3/mmc$, Z = 2) consists of hcp layers of O and Na atoms. $V(1)O_6$ octahedra form a Kagome; lattice, while $V(2)O_6$ octahedra form a face-sharing dimer. V(3) cations are five-fold coordinated to oxygen. The compound shows two structural phase transitions at 243K ($P6_3/mmc$ ---