

05.1-45 PHASE TRANSITION FROM A PARAMAGNETIC TO A MAGNETICALLY ORDERED CRYSTAL.

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On the basis of Landau's theory we have calculated changes of symmetry at a continuous phase transition of a paramagnetic crystal of symmetry $P6_3/mmc1'$ to magnetically ordered phases. The symmetry changes are induced by active representations connected with the wave vector $\vec{k} = \gamma \vec{b}_3$, $-0.5 < \gamma < 0.5$. These representations fulfil the reality condition, the Kovalev condition and the weak Lifshitz condition. We have considered two active representations which correspond to spins perpendicular to the C_6 axis. It has been proved

that there can appear two types of spin structures: /1/ with constant spin length, i.e. helical structures, and /2/ with varying spin length, i.e. sinusoidal structures. For the first case, formulae for the spiral structures which are valid for any value of γ from the interval $-0.5, 0.5$ have been given. We can thus obtain commensurate or incommensurate helical spin structures. With an appropriate value of γ we can obtain the helical structure of dysprosium crystal. In Landau's theory, the corresponding phase transition can be continuous. For the second case we give an example of a sinusoidal spin structure which is characteristic for neodymium crystal. The type of magnetic group to be assigned to a particular spin structure depends on the value of γ .

05.1-46 FERROELASTIC PHASES AND ORDER PARAMETER TREATMENT IN $Pb_3(P_{1-x}As_xO_4)_2$. By U. Bismayer, E. Salje⁺, A.M. Glazer and J. Cosier, Clarendon Laboratory, Parks Rd., Oxford OX1 3PU, UK.

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Lead phosphate and the isostructural mixed crystals of lead phosphate-arsenate exhibit ferroelastic transitions between the phases $R\bar{3}m$, $C2/c$ and $P2_1/c$. High precision measurements of optical birefringence and dielectric measurements revealed at temperatures below 100K in all compounds a further transition. In lead arsenate this probably corresponds to the transformation of $Pb_3(VO_4)_2$ to the acentric phase $P2_1$.

In $Pb_3(PO_4)_2$ the critical order parameter exponent β fits in with a multicomponent order parameter model with $q = 3$, $d = 2$ (Salje and Devarajan, J. Phys. C (1981) 14, L1029). Along with the results of infrared reflection spectroscopy, diffuse X-ray, neutron and Raman scattering, the precursor ordering behaviour indicates dynamical fluctuations in $Pb_3(PO_4)_2$ and a static intermediate phase in the mixed crystals.

The transition $C2/c - P2_1/c$ is interpreted in terms of a two-order-parameter theory, which clearly demonstrates how the first-order transition in pure $Pb_3(AsO_4)_2$ becomes smoother in $Pb_3(P_{0.2}As_{0.8}O_4)_2$.

U.B. acknowledges financial support from the Wissenschaftsausschuss der NATO through the DAAD.

05.1-47 STRUCTURES OF THE FERROELECTRIC AND PARAELECTRIC PHASES OF METHYLAMMONIUM TRICHLOROMERCURATE. By M. Körfner, H. Fuess and J.W. Bats, Institut für Kristallographie der Universität, Frankfurt am Main, Federal Republic of Germany

A first order ferro/paraelectric phase transition in $CH_3NH_3HgCl_3$ at 61°C was observed by differential scanning calorimetry, by birefringence and DK-measurements. The DSC-peak exhibits considerable structure and extends over about 1°C. The ferroelectric room temperature structure has space group $P3_2$, but shows three pseudo two-fold axes (Ben Salah et al., Z. anorg. allg. Chem. (1982) 493, 178). Further refinement was achieved by the introduction of two domains linked by a two-fold axis (R(F) decreased from 0.056 to 0.046). In the paraelectric phase, the structure is described in the monoclinic space group $C2$ ($a=13.818(2)$, $b=7.884(1)$, $c=9.734(3)$, $\beta=90.49(2)$). The polar three-fold axis is lost and one pseudo two-fold axis becomes a real one. Two Hg-atoms become symmetrically independent with drastically changed Hg-Cl distances as compared with the ferroelectric phase. Spectroscopic studies of the dynamics of the phase transition are in progress. The structures of the chemically related compounds $CH_3NH_3HgBr_3$ (space group $P2_1/m$; $a=7.985(2)$; $b=6.387(8)$, $c=8.728(3)$, $\beta=117.17(3)$) and $CH_3NH_3HgJ_3$ (space group $P2_1/n$; $a=9.089(4)$, $b=7.006(4)$, $c=14.817(11)$, $\beta=91.70(4)$) were also determined, but these compounds are not ferroelectric at room temperature.

05.1-48 A NEUTRON SCATTERING STUDY OF THE INCOMMENSURATE PHASE IN ALPO₄ (BERLINITE) NEAR THE α - β TRANSITION. By H. Arnold⁺, J. Bethke⁺⁺, G. Eckold⁺⁺⁺, Th. Hahn⁺, J. Min-Hua⁺⁺⁺; ⁺ Inst. für Kristallographie, RWTH Aachen, 51 Aachen, ⁺⁺ Inst. für Festkörperforschung, Kernforschungsanlage Jülich, 5170 Jülich, FRG; ⁺⁺⁺ Crystal Material Institut, Shandong University, Jinan Shandong, The Peoples Rep. of China.

Quartz and its isotype ALPO₄ (Berlinite) have many physical properties in common, especially the symmetry change at the α - β transition and the microdomain structure near the transition temperature. We report on our elastic neutron scattering results of the intermediate incommensurate phase of ALPO₄ existing in a temperature range of about 1.5 K between the α and the β phase. The experiments were performed on the triple axis spectrometer UNIDAS at the FRJ-2 reactor in Jülich using 0.25° collimation. Crystals with typical dimensions of 2.5 x 2.5 x 20 mm³ were grown under hydrothermal conditions. After having passed the α - β transition several times, satellite reflections were observed in the directions a^* , b^* and $a^* - b^*$ in various Brillouin zones. In particular, satellites corresponding to directions of the modulation vector q perpendicular to the reciprocal lattice vector Q exhibit large structure factors. The temperature dependence of q , which indicates the incommensurate character of this intermediate phase has been determined unambiguously. Within the temperature interval of 1.5 K the satellites display a linear shift from $q = 0.02$ up to $q = 0.038$ reciprocal units with increasing temperature.