

## 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  $\gamma$  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  $\gamma$  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  $\gamma$ .

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  $\beta$  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  $Pb_3(P_{0.2}As_{0.8}O_4)_2$ .

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05.1-47 STRUCTURES OF THE FERROELECTRIC AND PARAELECTRIC PHASES OF METHYLAMMONIUM TRICHLOROMERCURATE. By M. Körfer, 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  $ALPO_4$  (BERLINITE) NEAR THE  $\alpha$ - $\beta$  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  $ALPO_4$  (Berlinite) have many physical properties in common, especially the symmetry change at the  $\alpha$ - $\beta$  transition and the microdomain structure near the transition temperature. We report on our elastic neutron scattering results of the intermediate incommensurate phase of  $ALPO_4$  existing in a temperature range of about 1.5 K between the  $\alpha$  and the  $\beta$  phase. The experiments were performed on the triple axis spectrometer UNIDAS at the FRJ-2 reactor in Jülich using  $0.25^\circ$  collimation. Crystals with typical dimensions of  $2.5 \times 2.5 \times 20$  mm<sup>3</sup> were grown under hydrothermal conditions. After having passed the  $\alpha$ - $\beta$  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.