

PS11.05.19 TWIN DOMAINS AND PHASE TRANSITIONS OF KLiSO_4 . H. Klapper, Th. Hahn, Ch. Scherf, H.M. Park, G. Heger, Institut fuer Kristallographie, Rheinisch-Westfaelische Technische Hochschule, D-52056 Aachen, Germany.

We have investigated phase boundaries, twin formation and domain shapes during four phase transitions of KLiSO_4 in the temperature range 150K to 980K. Single-crystal plates were examined in-situ by polarisation-microscopy, synchrotron-radiation Laue topography and Lang X-ray topography.

The tetrahedral framework structure of KLiSO_4 exhibits a rich temperature polymorphism. In the room-temperature phase III (space group $P6_3$) four types of grown-in merohedral twins are distinguished. Heating above 708K from phase III and cooling below 949K from the high-temperature phase I leads to the intermediate orthorhombic phase II. Both transitions produce a dense twinning with three ferroelastic domain variants rotated by 120° around [001] (pseudo-hexagonal twins). In the "parent" phase I no twins are found, which confirms its hexagonal symmetry $P6_3/mmc$ or $P6_3/mc$. After the transition cycle III \rightarrow II \rightarrow III phase III shows an irregular domain arrangement with the same twin laws as the growth twins.

During cooling from phase III the sluggish transition into phase IV ($P31c$) starts at about 208K. The growth twins ($m // [001]$) of the hexagonal phase vanish and thin (0001) lamellae with the twin law $2 // [001]$ appear. Upon further cooling below 190K the pseudo-hexagonally twinned monoclinic phase V is formed. After re-transition into phase III the original grown-in twin pattern appears again (memory effect).

Crystal-structure analyses of phases I, II and V are in progress, based upon the group-subgroup relations of the phase transitions.

PS11.05.20 ANOMALOUS OF STRUCTURE AND PHASE TRANSITION OF PEROVSKITES. N. Kulagin, TU Kharkov, pr. Pravda 7 - 87, 310022 Kharkov, Ukraine

This report deals with a new phenomena in ABO_3 single crystals: disappear of ESR signal during 1200 - 3600 s for some doped SrTiO_3 crystals under 105K, anomalous of optical data for other crystals [1]. We study spectral properties: optical, ESR, X-Ray shift and Raman scattering connected with defests of structure of perovskites. For definite crystals, doped by V, Cr, Mn and another 3d- ions with $C = 10^{-3} - 10^{-2}$ wt % we registrated anomaly of optical and dielectric parameters. For some SrTiO_3 crystals we studied shift of T_c and so-called expansion phase transition [2]. There are calculated the electronic structure of clusters of doped and regular ions and defects for perovskites [3].

1. N. Kulagin, V. Sandulenko, L. Korostel. Proc. VIII Int. Conf. Ferroelect. Maryland. 1993. 428
2. N. Kulagin, D. Sviridov. Methods of Electronic Structure Calculations. Moscow. Nauka. 1986.
3. N. Kulagin, D. Sviridov. Introduction to Doped Crystals Physics. Kharkov. 1990.

PS11.05.21 PHASE TRANSITION IN DI-TETRAMETHYLAMMONIUM HEXAFLUORO-PLATINATE(IV). H. Küppers⁽¹⁾, C. Bruhn⁽²⁾, and W. Preetz⁽²⁾. ⁽¹⁾Mineralogisches Institut, ⁽²⁾Institut für Anorganische Chemie, Universität Kiel, D-24098 Kiel, Germany.

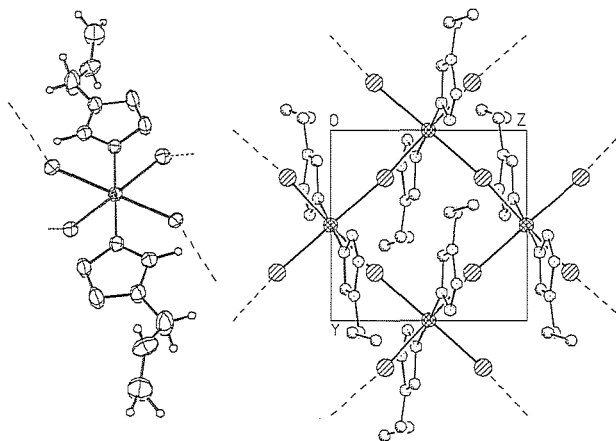
$(\text{TMA})_2[\text{PtF}_6]$ has been reported as being cubic ($Fm\bar{3}m$) and belonging to the $\text{K}_2[\text{PtCl}_6]$ type. Crystals grown at 5°C from a water-acetone solution exhibit quasi-cubic morphology (cube, octahedron, rhombic dodecahedron). Between crossed polarizers they show, however, interference colours in accord with tetragonal symmetry (tetragonal c axis pointing along one of the quasi-cubic axes). The refractive indices $n_o = 1.4788(6)$ and $n_e = 1.4768(6)$ were measured at 589 nm on a spindle stage. The double refraction (mea-

sured with an Ehringhaus compensator) amounts to $-0.0020(2)$ at room temperature and disappears, on heating, at $164(2)^\circ\text{C}$, following a parabolic decay with a critical exponent $\gamma = 0.58$. DTA measurements show a small endothermic peak at $163(2)^\circ\text{C}$. Twins or trillings are often observed with sharp {110} twin boundaries. Application of stress induces ferroelastic switching. In particular, uniaxial pressure along [100] causes the change from a to c.

Lattice parameters, referred to the quasi-cubic face-centred cell, determined at room temperature, differ only slightly : $a = 11.420(4)$, $c = 11.406(4)$ Å. A preliminary single crystal X-ray structure analysis shows only small deviations from the $\text{K}_2[\text{PtCl}_6]$ structure. Equatorial fluorine atoms have enlarged displacement parameters. The hydrogen atoms of the methyl groups are directed towards the fluorine atoms with distances $\text{C}\cdots\text{F} = 3.36$ Å.

PS11.05.22 MAGNETIC PROPERTIES AND STRUCTURE OF NEW COMPOUND DICHLOROBIS(1-ALLYLTETRAZOLE)COBALT(II). L.G. Lavrenova, V.N. Ikorskii, A.V. Virovets, N.V. Podberezskaya, G.A. Bikzhanova, S.V. Larionov, Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

The new complex compound of CoCl_2 with 1-allyltetrazole (altz) of composition $\text{Co}(\text{altz})_2\text{Cl}_2$ was prepared and its crystal structure (at 300 K) and magnetic properties in the 78-300 K range were investigated. $\text{Co}(\text{altz})_2\text{Cl}_2$ shows antiferromagnetic ordering with weak ferromagnetism, the Neel temperature is 102 K. The magnitude of spontaneous magnetic moment at 80 K is $665 \text{ Gcm}^3\text{mol}^{-1}$



In the crystal $\text{Co}(\text{altz})_2$ units are connected by symmetrical Cl bridges into layers as in isostructural $\text{Cu}(\text{altz})_2\text{Cl}_2$ (*Zhurnal Strukturnoi Khimii (Russian)*, 37(1996) 330). Co-Cl and Co-N distances are 2.538(1) and 2.085(3) Å respectively, angle Co-Cl-Co is $143.22(4)^\circ$. The structure at 300 K (and probably at lower temperature) is quasi-two-dimensional because the layers are separated by long van der Waals contacts ($\text{C}\cdots\text{C}3.55$ Å). At the same time in Cu analog the ferromagnetic ordering takes place (the Curie temperature is 10 K, the magnetization at 4.3 K in the 10.9 kOe field is $5523 \text{ Gcm}^3\text{mol}^{-1}$, *Zhurnal Neorgan. Khimii (Russian)*, 38(1993) 1517).