

## 21-Crystallography at Non-Ambient Temperatures and/or Pressures; Phase Transitions

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about one sixth of those at 296 K, and that of S atom reduces to one tenth (Table 1).

Table 1. Unit cell parameters and atomic positions of  $K_2SO_4$  at 15 K and 296 K

Unit cell parameters at 15 K				
	a (Å)	b (Å)	c (Å)	
	5.7226(4)	9.9985(4)	7.4218(3)	
Atomic position at 15 K				
atom	x	y	z	$U_{eq}$ (Å <sup>2</sup> )
K1	0.25	0.58951(5)	0.67139(6)	0.00258(8)
K2	0.25	0.29720(5)	-0.01118(9)	0.00218(8)
S	0.25	0.57985(5)	0.23261(7)	0.00086(10)
O1	0.25	0.5828(2)	0.0344(2)	0.0047(3)
O2	0.25	0.4399(2)	0.2939(2)	0.0037(3)
O3	0.0390(2)	0.6486(1)	0.3015(2)	0.0038(2)
R=0.037 wR=0.034				
Unit cell parameters at 296 K				
	a (Å)	b (Å)	c (Å)	
	5.7704(3)	10.0712(9)	7.4776(4)	
Atomic position at 296 K				
atom	x	y	z	$U_{eq}$ (Å <sup>2</sup> )
K1	0.25	0.58936(7)	0.6742(1)	0.0161(1)
K2	0.25	0.29544(7)	-0.01082(9)	0.0138(1)
S	0.25	0.58006(7)	0.23300(9)	0.0082(1)
O1	0.25	0.5829(3)	0.03719(3)	0.0251(7)
O2	0.25	0.4426(2)	0.2970(3)	0.0188(6)
O3	0.0421(3)	0.6480(2)	0.3005(2)	0.0199(4)
R=0.045 wR=0.043				

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PS-21.02.09 TIME-RESOLVED X-RAY POWDER DIFFRACTION STUDY OF POLYMORPHISM IN COBALT NITRATE HEXAHYDRATE AND PHASE TRANSFORMATIONS AT LOW TEMPERATURES. By J. Plevert\*, H. Hashizume and D. Louer<sup>1</sup>, Tokyo Institute of Technology, Japan, <sup>1</sup>University of Rennes, France.

Three polymorphs of  $Co(NO_3)_2 \cdot 6H_2O$  are known to exist at low temperatures. When the room-temperature phase is cooled at high cooling rates, the low-temperature phase is produced by a burst effect in the crystal during the martensitic transformation. For slow cooling rates, an intermediate phase is obtained (P. Pouillen & al. (1965). *C. R. Acad. Sc. Paris*, 260, 6861). Moreover the hygroscopic properties of the sample are an important factor of the phase stability. The modification of environmental conditions brings a new phase.

Powder patterns recorded at low temperatures using a position sensitive detector provide information about the kinetics of the martensitic transformation. The structural information of different phases obtained from these data provides the relationship between the polymorphs, and allows the driving force of the phase change to be determined.

### 21.03 - Phase Transitions in Crystals

MS-21.03.01 The Landau-free-Energy expansion for the phase transition in liquid crystals

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The theoretical investigation of the phase transition between the different liquid crystal smectic phases is performed after applying the Landau approach. The descriptions of the free energy are given according to the Landau-Lifshitz condition. The X-ray flat patterns during the phase transition are discussed.

The analysis shows a wide variety of the symmetry allowed phase transitions in ordered smectics. The results for the space symmetry group are presented. Beside this, some experimentally detected smectic phases, e.g. the hexatic smectic ( $D_{6h}$ ), smectic F and I ( $C_{2h}$ ), unstuck smectic B ( $D_{6h}^1$ ), smectic E ( $D_{2h}^9$ ), smectic J and G ( $C_{2h}^3$ ), smectic H and K ( $C_{2h}^5$ ), are discussed especially.

As the first step here, only the transitions with change of space group are presented. It should be pointed out that some transitions may lead to the phases with the same symmetry group and another unit cell.

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MS-21.03.02

A SOLID-SOLUTION THEORY OF ANESTHETIC INTERACTION WITH MEMBRANES, By Y. Suezaki, Physics Laboratory Saga Medical School, Saga 849, Japan.

Anesthetics (or any other small molecules) depress the temperature of the main phase transition of phospholipid bilayers. Certain anesthetics widen the temperature span of the transition, whereas others do not. The widening in the first-order phase transition is intriguing.

In this report, the effect of additive molecules on the transition temperature and its temperature span were explained by the solid-solution theory. By assuming the coexistence of the liquid-crystal and solid-gel phases of lipid membranes at phase transition, the phase boundary is determined from the distribution of anesthetic molecules between the liquid-crystal membrane versus water and the solid-gel membrane versus water.

The theory shows that when the lipid concentration is large or when the lipid solubility of the drug is large, the temperature width of the transition increases, and vice versa. Highly lipid-soluble molecules such as long-chain alcohols and volatile anesthetics, increase the temperature width of the phase transition when the lipid:water ratio is large, whereas highly water-soluble molecules, such as methanol and ethanol, do not. The aqueous phase serves as the reservoir for anesthetics. Depletion of the additive molecules from the aqueous phase is the cause of the widening. When the reservoir capacity is large, the temperature width does not increase. The theory also predicts asymmetry of the specific heat profile at the transition. (Y. Suezaki, T. Tatara, Y. Kaminoh, H. Kamaya and I. Ueda, *Biochim. Biophys. Acta*, 1990, 1029, 143. and Y. Suezaki, H. Kamaya and I. Ueda, *Phase Transitions*, 1990, 29, 37.)