

Pressure-induced structural transformation in potassium stanichloride

P KISTAIAH, K SATHYANARAYANA MURTHY,
LEELA IYENGAR and K V KRISHNA RAO

Department of Physics, University College of Science, Osmania University,
Hyderabad 500 007, India

MS received 14 August 1980; revised 29 September 1980

Abstract. Pressure-induced structural transformation in potassium stanichloride has been studied by x-ray diffraction at room temperature. The change in the diffraction pattern started at about a pressure of 15 kbar and continued upto 50 kbar. The pattern recorded at about 50 kbar could be indexed basing on an orthorhombic lattice, with lattice parameters $a=7.32$, $b=7.02$ and $c=8.02$ Å.

Keywords. Potassium stanichloride; structural transformation; x-ray diffraction; high pressure.

1. Introduction

Potassium stanichloride (K_2SnCl_6), a member of A_2MX_6 -hexahalometallates, crystallises in the cubic face-centered antifluorite structure of space group $O_h^5 [Fm\bar{3}m]$ at room temperature and atmospheric pressure (Dickinson 1922; Brill *et al* 1974; Lerbscher and Trotter 1976; Ihringer 1977). The Sn atoms occupy an fcc lattice and are surrounded by Cl_6 octahedra, which are oriented according to the cubic symmetry. The K atoms form a primitive cubic lattice with $a/2$, which is shifted $1/4$ along the room diagonal. The crystal undergoes two structural phase transitions from its cubic room temperature phase to a lower symmetry at low temperatures (Morfee *et al* 1960; Sasane *et al* 1970; Jeffrey 1972; Winter and Rössler 1976; Winter *et al* 1976; Boysen *et al* 1976). Until recently, according to neutron-scattering and x-ray measurements (Boysen and Hewat 1978; Boysen *et al* 1976), phase transitions were considered to occur from the cubic room temperature phase O_h^5 to a tetragonal structure of space group D_{4h}^6 at $T_{c1} = 261^\circ K$ and to a monoclinic structure of space group C_{2h}^5 at $T_{c2} = 255^\circ K$. More recent x-ray scattering experiments by Kugler *et al* (1979) and Brillouin-scattering experiments by Henkel *et al* (1980b), however, do not support this result. A symmetry change from O_h^5 to the orthorhombic structure of space group D_{2h}^3 at T_{c1} and the monoclinic structure of space group C_{2h}^5 below T_{c2} are found to be most compatible with their experimental results. Recent Raman-scattering experiments on K_2SnCl_6 under hydrostatic pressure by Henkel *et al* (1980a) showed that the crystal becomes orthorhombic at room temperature under a pressure of about 45 kbar. However, no x-ray studies on the structural changes of this compound under pressure at room temperature are reported so far. In an effort to study the structural changes