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CHANGES IN CRYSTAL LATTICE PARAMETERS OF PENTAERYTHRITOL AT PRESSURES UP TO 10,000 kg/cm^2

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An x-ray study has been made of the change in the crystal lattice parameters a and c of pentaerythritol $C(CH_2OH)_4$, which has a tetragonal structure with a = 6.10 A and c = 8.73 A, resulting from direct action of quasihydrostatic pressures up to 10,000 kg/cm^2 at room temperature. The lattice parameters had the following values at 9000 kg/cm^2: a = 5.99 A and c = 8.46 A. A phase transformation of pentaerythritol was observed in the pressure range 4200-5600 kg/cm^2 from a jump in the parameters a and c and in the volume (~2.6%), the crystal structure remaining the same both below and above the transition pressure.

A good description of the behavior of pentaerythritol under pressure is given by two empirical equations of state of third degree in the pressure having the form:

$$\text{before transition} \quad -\frac{\Delta V}{V_0} = 1.584 \cdot 10^{-5}P - 2.380 \cdot 10^{-9}P^2 + 0.330 \cdot 10^{-13}P^3,$$

$$\text{after transition} \quad -\frac{\Delta V}{V_0} = 2.404 \cdot 10^{-5}P - 3.848 \cdot 10^{-9}P^2 + 2.202 \cdot 10^{-13}P^3,$$

Above the transition pressure, pentaerythritol shows an anomalous compressibility, in that the compressibility increases with increase in pressure.

1. The apparatus described in [1] for making x-ray studies at high pressures up to 18,000 kg/cm^2 has been used in the present work to investigate the changes in the crystal lattice parameters of pentaerythritol occurring under pressure. The high pressure chamber used in the apparatus was a beryllium vessel of new and original form, which could be supported in a reliable way. A special system for adjusting and testing the x-ray chamber was provided. The construction of the apparatus is also such as to make it possible to rotate the sample under pressure.

The apparatus is comparatively simple in construction the pressure inside the chamber can be measured within relatively narrow limits, it is portable, and the film can be changed without losing pressure. The accuracy of the pressure measurements in the apparatus has been found from a considerable number of calibrating experiments and is 2% of the measured pressure (up to 10,000 kg/cm^2). A diagram of the experimental apparatus is shown in Fig. 1.

Pentaerythritol was chosen for the study because, like many organic crystals [2], a considerable change in volume was to be expected at high pressures.

Pentaerythritol $C(CH_2OH)_4$ belongs to the tetragonal system and has an elementary cell with a = 6.10 A and c = 8.73 A. Z (the number of molecules in the cell) = 2, the Fedorov group is $S_4^2(I\bar{4})$, and the symmetry of the molecule, both inherent and in the crystal, is $\bar{4}$ [3]. Very pure pentaerythritol was used in the present experiments. The samples were made from coarse crystalline pentaerythritol powder by selecting perfectly transparent crystals with dimensions from 0.5 to 3 mm and grinding them fine enough to give continuous x-ray lines without rotating the sample. The pentaerythritol samples were pressformed into small cylinders 0.8 mm in diameter and 4 mm high.

2. The present experiments were made with a beryllium chamber (used repeatedly under pressure) having an internal cylindrical channel with a diameter of 1.215 mm.