

Change in the Parameters  $\underline{a}$  and  $\underline{c}$  of pentaerythritol under pressure\*

Pressure, P, kg/cm <sup>2</sup>	Lattice parameters, A	
	$\underline{a}$	$\underline{c}$
1800	6.07	8.63
3000	6.07	8.58
4200	6.07	8.58
5600	6.01	8.52
6000	6.01	8.52
7200	6.01	8.50
7800	6.00	8.49
9000	5.99	8.46

\*Here  $\underline{a}$  is found with an accuracy of  $\pm 0.02$  A, for  $\underline{c}$ ,  $\pm 0.03$  A.

2 and 3 show graphs of the above polynomials and the experimental points.

It may be seen from the graphs that the compressibility is greatest in the direction in which the intermolecular distances are greatest and hence the binding forces are weaker.

At a pressure of 9000 kg/cm<sup>2</sup>, the total change in the parameter  $\underline{c}$  is 2.5 times greater than the corresponding change in the parameter  $\underline{a}$ , and the ratio  $\underline{c}/\underline{a}$  changed at the same time from the value 1.43 at atmospheric pressure to the value of 1.41.

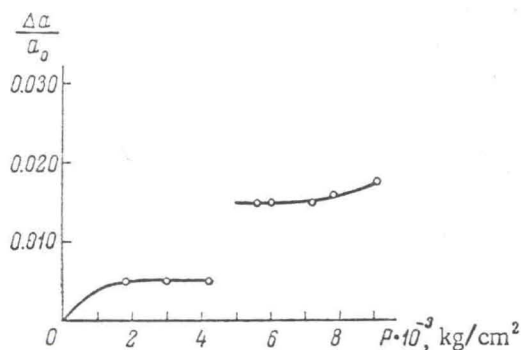


Fig. 2. Linear compressibility,  $\Delta a/a_0$ , of  $C(CH_2OH)_4$  as a function of pressure.

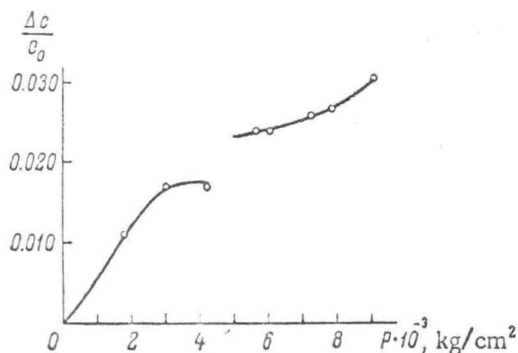


Fig. 3. Linear compressibility,  $\Delta c/c_0$ , of  $C(CH_2OH)_4$  as a function of pressure.

The equations for  $\Delta V/V_0$  as a function of P in the pressure ranges given are:

$$-\frac{\Delta V}{V_0} = 1.584 \cdot 10^{-5} P$$

$$-2.380 \cdot 10^{-9} P^2 + 0.330 \cdot 10^{-13} P^3,$$

$$-\frac{\Delta V}{V_0} = 2.404 \cdot 10^{-5} P$$

$$-3.848 \cdot 10^{-9} P^2 + 2.202 \cdot 10^{-13} P^3.$$

It may be seen from the data that in the pressure range 4200-5600 kg/cm<sup>2</sup> there is a jump in the lattice parameters  $\underline{a}$  and  $\underline{c}$  and in the volume ( $\sim 2.6\%$ ) which is greater than the error of the measurements. When calibrating the apparatus with a pentaerythritol sample as well as when taking the x-ray diagrams, a jump in volume was observed from the dynamometer readings at a pressure close to 5000 kg/cm<sup>2</sup>.

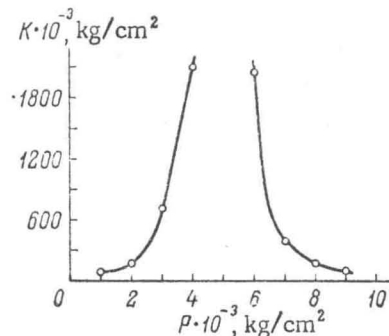


Fig. 4. Bulk modulus of  $C(CH_2OH)_4$  as a function of pressure.

Analysis of the x-ray patterns showed that the crystal structure of pentaerythritol stays the same below and above the transition pressure, and the volume jump is probably to be explained by an increase in packing density of the pentaerythritol molecules in the crystal lattice.

Analysis of the equations giving  $\Delta a/a_0$  and  $\Delta c/c_0$  as a function of pressures shows that the change in compressibility along the  $\underline{a}$  and  $\underline{c}$  axes is of a different nature below and above the transition pressure. Below the transition pressure (4200 kg/cm<sup>2</sup>) the compressibility drops off in a normal way as the pressure is increased, while above the transition pressure the compressibility increases with increasing pressure. This peculiarity in the behavior of pentaerythritol we have shown in Fig. 4 for the bulk modulus K, which is the reciprocal of the compressibility. It turned out that in contrast to the bulk moduli of metals and some ionic crystals [5, 6] the change in the K modulus of pentaerythritol with pressure is nonlinear and is discontinuous in the transition region.

The experimental data obtained in this work on the pressure dependence of the volume V and the bulk modu-

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