

ground state energy  $E_0$ , distance  $2\zeta$ ) in case of  $q^2 \gg 1$ , the tunneling energy is given by [6, 7]

$$\Omega = \frac{h^2}{\sqrt{\pi} m \zeta^2} q^3 \exp(-q^2); \quad q^2 \equiv \frac{2 m E_0 \zeta^2}{h^2}. \quad (6)$$

Thus,

$$\frac{d\Omega}{d\zeta} = -(2q^2 - 1) \frac{\Omega}{\zeta}. \quad (7)$$

By substituting (4), (5), (6), and (7) in (3) we find

$$\frac{dT_c}{dp} = \frac{T_c}{\zeta} \frac{d\zeta}{dp} \left[ \frac{kT_c J}{2\Omega^2} \left( \sinh \frac{\Omega}{kT_c} \right)^2 + (2q^2 - 1) \left( \frac{kT_c}{2\Omega} \sinh \frac{2\Omega}{kT_c} - 1 \right) \right]. \quad (8)$$

We introduce  $\zeta^{-1} d\zeta/dp = -\alpha S_1$  with  $S_1 = a^{-1} da/dp = s_{11} + s_{12} + s_{13}$ , and  $\alpha = (a/\zeta) d\zeta/da$ ,  $a$  being the lattice constant, and  $s_{ij}$  the elastic compliances. Finally, after eliminating  $J$  by means of equation (2) we obtain

$$\frac{dT_c}{dp} = -\alpha S_1 T_c \left[ 2 + (2q^2 + 1) \left( \frac{kT_c}{2\Omega} \sinh \frac{2\Omega}{kT_c} - 1 \right) \right]. \quad (9)$$

The second term in the square bracket of equation (9) describes the effect of proton tunneling on the shift of  $T_c$  with pressure. It is a positive quantity and may be neglected under the condition  $\Omega/kT_c \ll 1$  which can be considered to be fulfilled for the deuterated crystals.

Since  $\alpha$  is a positive quantity ( $d\zeta/da > 0$ ), the transition temperature  $T_c$ , according to equation (9), is always shifted towards lower temperatures with pressure. At given  $T_c$  the shift increases with increasing  $\Omega$ . In Fig. 5, the pressure shift  $-dT_c/dp$  is represented as a function of  $T_c$  according to equation (9), with  $\alpha S_1 = 9.4 \times 10^{-3} \text{ kbar}^{-1}$ . This value has been chosen so that for  $\text{KD}_2\text{PO}_4$  ( $\Omega/kT_c \ll 1$ ) equation (9) gives  $dT_c/dp = -3.9 \text{ deg/kbar}$  ( $T_c = 208 \text{ }^\circ\text{K}$ ) which was measured by Samara [2]. The value of  $\alpha S_1$  found for  $\text{KD}_2\text{PO}_4$  can also be taken in good approximation for  $\text{KH}_2\text{PO}_4$ . Then equation (9) can be used to determine  $\Omega$  from the measured value of  $dT_c/dp$ . The necessary relation between  $q$  and  $\Omega$  is given by equation (6). For  $\text{KH}_2\text{PO}_4$  we use  $\zeta = 0.19 \text{ \AA}$  [13] and obtain  $\Omega/k = 79 \text{ }^\circ\text{K}$  or  $\Omega = 1.09 \times 10^{-14} \text{ erg}$ . This

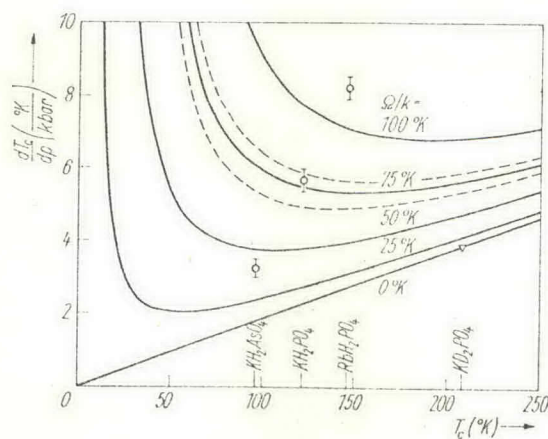


Fig. 5. Pressure shift  $-dT_c/dp$  as a function of the phase-transition temperature  $T_c$  according to (9) for various values of  $\Omega$ . The curves were fitted to the measured value [2] for  $\text{KD}_2\text{PO}_4$  (cf. the text). For the parameter value  $\Omega/k = 75 \text{ }^\circ\text{K}$  also curves with  $\zeta = 0.15 \text{ \AA}$  and  $\zeta = 0.25 \text{ \AA}$  in dashed lines are given in addition to the curve with  $\zeta = 0.19 \text{ \AA}$ .