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

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

Thus,

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

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

$$\frac{\mathrm{d}T_c}{\mathrm{d}p} = \frac{T_c}{\zeta}\frac{\mathrm{d}\zeta}{\mathrm{d}p}\left[\frac{kT_c\, J}{2\,\Omega^2}\left(\sinh\frac{\Omega}{kT_c}\right)^2 + (2\,q^2 - 1)\left(\frac{kT_c}{2\,\Omega}\sinh\frac{2\,\Omega}{kT_c} - 1\right)\right]. \tag{8}$$

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

$$\frac{\mathrm{d}T_c}{\mathrm{d}p} = -\alpha\, S_1\, T_c\left[2 + (2\,q^2 + 1)\left(\frac{kT_c}{2\,\Omega}\sinh\frac{2\,\Omega}{kT_c} - 1\right)\right]. \tag{9}$$

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 α is a positive quantity ($\mathrm{d}\zeta/\mathrm{d}a > 0$), 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 Ω. In Fig. 5, the pressure shift $-\mathrm{d}T_c/\mathrm{d}p$ is represented as a function of T_c according to equation (9), with $\alpha\, S_1 = 9.4 \times 10^{-3}$ kbar^{-1}. This value has been chosen so that for KD_2PO_4 ($\Omega/kT_c \ll 1$) equation (9) gives $\mathrm{d}T_c/\mathrm{d}p = -3.9$ deg/kbar ($T_c = 208$ °K) which was measured by Samara [2]. The value of $\alpha\, S_1$ found for KD_2PO_4 can also be taken in good approximation for KH_2PO_4. Then equation (9) can be used to determine Ω from the measured value of $\mathrm{d}T_c/\mathrm{d}p$. The necessary relation between q and Ω is given by equation (6). For KH_2PO_4 we use $\zeta = 0.19$ Å [13] and obtain $\Omega/k = 79$ °K or $\Omega = 1.09 \times 10^{-14}$ erg. This

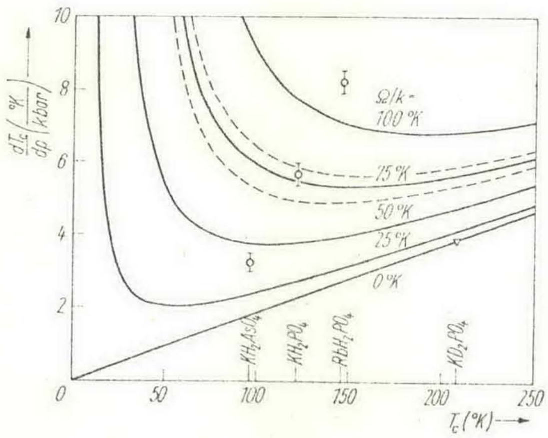

Fig. 5. Pressure shift $-\mathrm{d}T_c/\mathrm{d}p$ as a function of the phase-transition temperature T_c according to (9) for various values of Ω. The curves were fitted to the measured value [2] for KD_2PO_4 (cf. the text). For the parameter value $\Omega/k = 75$ °K also curves with $\zeta = 0.15$ Å and $\zeta = 0.25$ Å in dashed lines are given in addition to the curve with $\zeta = 0.19$ Å