ISOTOPIC EFFECT OF VIBRATIONS OF H-BONDS IN CRYSTALS. THE THREE-DIMENSIONAL MDEL

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On the basis of the three-dimensional model for description of the H-bonds in crystals the stretching and banding vibrations of protons (deuterons) were theoretically investigated. The dependencies of frequencies these vibration on the hydrogen bond lengths $R_{O...O}$ for a wide series of hydrogen-containing crystals, for the cases when $R_{O...O} < R_c$ and $R_{O...O} > R_c$. The R_c value corresponds to the critical magnitude of the hydrogen bond length when two-minimum hydrogen bond transforms into one-minimum bond. It is shown that observed increasing of the banding vibration frequency with decreasing of the hydrogen bond length, what caused by some rising of hydrogen bonds in the transversal direction. For range hydrogen bond lengths $R_{O...O} \geq R_c$ the frequency of stretching vibration downs to value $5 \cdot 10^2$ cm^{-1}, what is explained by transformation of proton potential $U(x)$ into one-minimum: $U(x) = a^4 D_0 x^4/4$, where a, D_0 are potential parameters. It is obtained that the critical value Rc is some less than corresponding value, which was obtained in[a]. It is possible due to the introduction of transversal functions.

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[a] S. Tanaka, Phys. Rev. B, **42** 10488 (1990).