

A THREE-DIMENSIONAL MODEL OF H-BOND  
AND THE GEOMETRIC ISOTOPIC EFFECT

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The geometric isotopic effect in hydrogen-containing crystals of the KDP-type is investigated. A mechanism of changes of the hydrogen bonds lengths under the deuterium substitution is proposed. It is shown that (in the framework of the three-dimensional model for hydrogen bonds based on the Einstein approximation for anharmonic oscillators) the correspondence between experimental and theoretical data can be achieved if one takes into account the interactions between the neighboring chains of H-bonds in a crystal.