

## Hydrogen bond simulation in molecular crystals of tyrosine

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**Keywords:** amino acids, tyrosine,  $\alpha$ -amino- $\beta$ -paraoxyphenylpropionic acid, hydrogen bond, intermolecular interaction, simulation.

### Abstract

The problem of the study of hydrogen bonds in biomolecules and living systems is important. Among the drugs, doctors emphasize substances of natural origin involved in metabolic processes. Such compounds include amino acids, peptides, vitamins, enzymes, macro- and microelements, and other biologically active substances, many of which are capable of forming hydrogen bonds. Amino acids and their derivatives are drugs of metabolic pharmacotherapy, characterized by low toxicity and severity of side effects. They also have virtually no allergenic effect, which makes them promising for the creation of drugs or their modifications. The instability of the hydrogen bond can significantly affect the state of pharmaceutical drug containing, for example, amino acids, during their storage, transportation or technological processing. One of the methods for studying the nature and determining the strength of hydrogen bonds is quantum chemical simulation. The calculation of the interaction energy in the studied molecular associate and its decomposition have been carried out according to Morokuma's method (HF/6-31G (PC GAMESS)). The evaluation of such energy components as electrostatic, exchange repulsion, polarization, charge transfer, mixing is given. The main contribution to the interaction energy comes from the electrostatic component. All the studied models have the same distribution of the components of the interaction energy in order of magnitude. Significant difference in the interaction energy in two model systems was noted, that could be explained by different geometry of hydrogen bonds. The comparison of received data made it possible to conclude that there are three types of hydrogen bonds in the molecular tyrosine crystal, which differ from each other in energy and geometry.

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