THEORETICAL STUDY OF PROTON EXCHANGE IN AMINOACETIC ACID DIMERS

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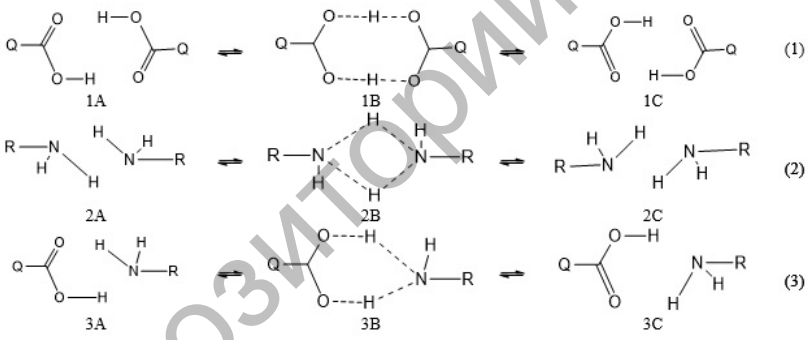
The molecule of aminoacetic acid has in its structure two protolytic reaction centers: a carboxyl group with acidic properties and an amino group with basic properties. Due to this aminoacetic acid can forms dimers caused by hydrogen bond [1]. The structure of some dimers is favorable for the process of intracomplex proton exchange. It was interesting to determine the most ideally structure for proton exchange in amino acetic acid dimers by quantum-chemical methods.

Geometries and energy parameters for three main types (1-3) of dimers were obtained at the 3-21G UHF *ab initio* level:



where Q – $-CH_2-NH_2$; R – $-CH_2-COOH$.

Simulation of the intermolecular proton exchange process in these dimers was carried out with the help of Quadratic Synchronous Transit approach (QST2) and Intrinsic Reaction Coordinate procedure (IRC). The activation energy of the forward ($E_{act\rightarrow}$) and reverse ($E_{act\leftarrow}$) protolytic processes was estimated for dimers 1-3. It was found that the activation energy was: for dimer 1 $E_{act\rightarrow}$=26 kJ/mol and $E_{act\leftarrow}$=34 kJ/mol; for dimer 2 $E_{act\rightarrow}$=244 kJ/mol and $E_{act\leftarrow}$=236 kJ/mol; for dimer 3 $E_{act\rightarrow}$=47 kJ/mol and $E_{act\leftarrow}$=36 kJ/mol. It is clear from the obtained data that the most favorable for proton exchange structures are dimers 1 and 3 in which carboxyl and amino groups are involved in hydrogen bonding.

References:

1. Kutzhanova K.Zh., Pustolaikina I.A., et al. (2016) *Bulletin of the University of Karaganda-Chemistry*, 4(84), 33-37.