QUANTUM-CHEMICAL MODELING OF PROTOLYTIC INTERACTION BETWEEN AMMONIA AND ACETIC ACID

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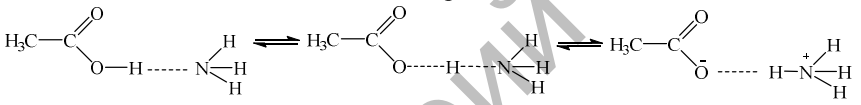
Intermolecular interaction between ammonia and acetic acid has protolytic nature. Acetic acid is capable to be a donor of protons, while ammonia is capable to accept protons. These small and well-studied particles are convenient objects for studying the mechanism of protolytic interaction. The purpose of this study was to simulate the elementary act of protolytic reaction by the sample of interaction between ammonia and acetic acid using modern methods of quantum chemistry.The scheme of protolytic interaction between ammonia and acetic acid can be presented as follows:



HBMC TS HBIC

Protolytic interaction begins from the formation of hydrogen bonding molecular complex (HBMC) between ammonia and acetic acid, then it transforms in to transition state (TS) and finally gives hydrogen bonding ionic complex (HBIC).

Calculations were carried out by ab initio 6-31G UHF method with the help of Gaussian 2009 [1]. Solvent (water) was counted using a macroscopic CPCM model. Molecular and ionic complexes were identified quantum-chemically as a result of calculations with full optimization of all geometric parameters. The Quadratic Synchronous Transit approach (QST2) was used for search of transition state (TS). The Intrinsic Reaction Coordinate procedure (IRC) was applied to calculate the sloping along the reaction coordinate from the transition state towards reactants (HBMC) and reaction products (HBIC).

Reduction of the hydrogen bridge length ($\Delta r(ON)=0.1$ Å) during the proton transfer process was noted. The activation energy of the proton transfer reaction was determined as the difference in the total energies of reactants (HBMC) and transition state (TS). The size of quantum-chemically estimated activation energy ($\Delta E_{act.}=15.75$ kJ/mol) is in a good agreement with experimental value of hydrogen bond energy, which does not exceed 40 kJ/mol.

References:

1. FRISCH, M. J., TRUCKS, G. W., SCHLEGEL, H. B., et al. 2009. Gaussian 09, Revision C.01. - Gaussian Inc., Wallingford CT.

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