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Data Article

Density functional theory investigation of inter and intramolecular hydrogen bonded complexes of 2-ethanolamine with water

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ABSTRACT

Hydrogen bonding interaction in 1:1 complexes between 2-Aminoethanol (AE) and water is investigated using DFT methods. Six low lying conformers of AE, which are intramolecular hydrogen bonded, are selected for the binary complex formation with water. Considering all possible binding motifs, a total of 19 different complexes involving various types of intermolecular hydrogen bonding are obtained at DFT-D level and 20 complexes at B3LYP level of calculation. During binary complex formation with water molecule, the intramolecular hydrogen bond is removed in most complexes and intermolecular hydrogen bonds are formed. In few cases, structural deformation results for accommodating water molecule for generation of intermolecular hydrogen bonds. The natural bond orbital (NBO) analysis and atoms in molecules (AIM) theory have been applied to understand the nature and strength of interaction present in AE-water complexes.

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Specification table

Subject area	Computational chemistry
Compounds	2-ethanol amine water complex
Data category	computational simulations
Data acquisition format	Quantum mechanical Density functional theory calculation
Data type	Simulated and analyzed
Procedure	All calculations are carried out using the Firefly QC package. The isolated geometries of the intramolecular hydrogen bonded AE, and their various binary complexes with water are fully optimized by the density functional theory (DFT) and density functional theory with dispersion correction (DFT-D) method using 6-311++G(2d, 2p) basis set. The stabilization energy between the partners in each complex at the energetic minimum was calculated using the super-molecule method. The interaction energy is further corrected for zero point vibrational energy. Bader's AIM Theory is used to investigate the electronic densities and intermolecular hydrogen bonding interactions in the binary complexes. Furthermore, to evaluate the direction and magnitude of the donor-acceptor interactions, the natural bond orbital (NBO) analysis for all the complexes has been performed using NBO 5.0 program.
Data accessibility	Available with this article only.

1. Rationale

Hydrogen bonding is an attractive interaction between a donor and an acceptor. The donor atoms are generally electronegative compared to hydrogen and acceptor atoms possesses unshared lone pair electrons [1–2]. Hydrogen bond play vital roles in biomolecular structures, self-assembly, crystal packing, supramolecular chemistry and many other fields [3–6]. Several important aspects of biological processes such as selective binding, molecular recognition and physicochemical properties are greatly influenced by hydrogen bonding interactions. Hydrogen bonding interactions of aromatic side chains govern the structure of proteins and the catalytic abilities of enzymes [7–9]. Understanding these interactions at molecular level imparts knowledge about the biological processes and functional structures of biomolecules. The study of hydrogen bonding interactions has created enormous interest, and became more and more important in research for several decades. A wealth of information can be found on hydrogen bonds in the literature [10–16]. It is extremely important as well as challenging to obtain quantitative information of hydrogen bonding interactions using accurate quantum mechanical calculations.

Hydrogen bonding interactions in multifunctional molecules, which have many sites to participate in hydrogen bonding interactions is a very interesting subject to investigate. These molecules are often stabilized by intramolecular hydrogen bonds between various available sites. Most often during the formation of binary complexes, these intramolecular hydrogen bonds break and result in a dramatic change of conformation. These interactions sometimes alter the relative stabilities of the conformers [17–19].

In this scenario 2-Aminoethanol, (AE), containing both -NH_2 and -OH functional group is an interesting molecule. The amino and hydroxyl groups simultaneously can behave as H-bond donor and acceptor and may involved in various types of intra and intermolecular hydrogen bonding. This molecule is found to be stabilized by strong intramolecular hydrogen bond [20–21]. In spite of being a simple molecule, it is an important constituent of some relevant biological systems. The backbone of many important systems such as ephedrine, pseudoephedrine, and 2-amino-1-phenylethanol exhibiting conformational changes upon complexation, consist of aminoethanol molecule [17–19]. Hence AE can act as the simplest model to study those systems extensively. AE has also received considerable attention due to its CO_2 capture properties to reduce the global warming problem [22–24]. Therefore, conformational analyses of isolated AE and its complexes are having theoretical as well as practical importance.

AE has been studied extensively by theory, experiment and also by combination of both methods [20–44]. Microwave [30–31], infrared [20,32] and photoelectron [33] spectroscopic studies suggest that in gas phase, this molecule exists predominantly in the Gauche conformer. Formation of intramolecular hydrogen bonds heavily influences the structural and spectroscopic parameters of this molecule and plays decisive role in stability of the conformers. The conformers without intramolecular H-bonds are higher in energy and are less populated in the gas phase.