HYDROGEN BONDING IN THE SYSTEM 3-AMINOPROPANOL - WATER

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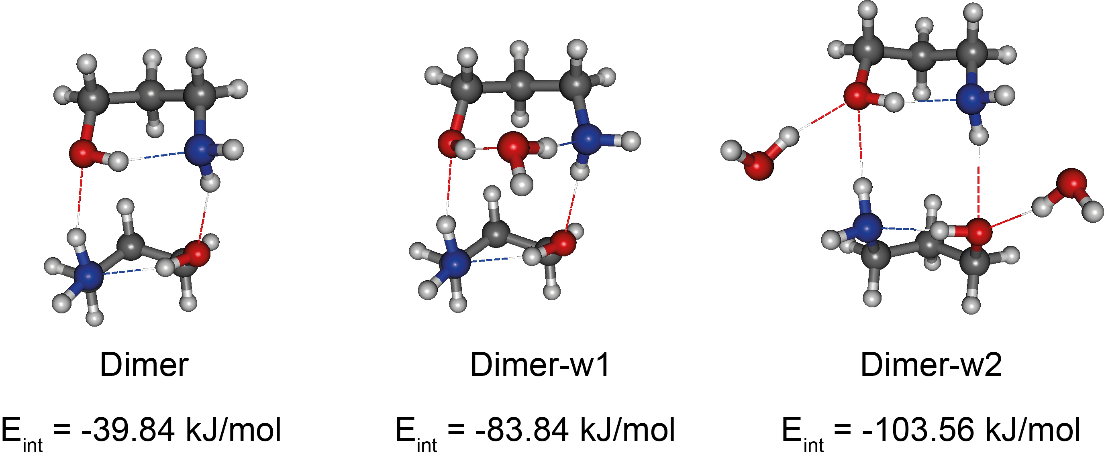
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**Abstract.**

Hydrogen bonds are well known to be formed to stabilize water, alcohols and other H-bond containing solvents. 3-Aminopropanol (3AP) is an aminoalcohol with both NH and OH groups acting as donor and acceptor in water. This computational study deals with different clusters of the system 3AP-water and answers the question what type of clusters are formed by hydrogen bonding and how they are stabilized.

The most stable conformers of the 3AP monomer were used to build 3AP-3AP dimers. In order to get trimers and tetramers, one or two water molecules were added at different positions around the dimer forms. Geometry optimization was performed using the MØeller-Plesset perturbation theory of second order using the method MP2/6-311++G(d,p). Counterpoise correction for the basis set superposition error was taken into account in the calculation. To compare with experimental literature data, frequency calculations were carried out to obtain vibrational data of the OH and NH bonds.

In this presentation, I will discuss the geometries of the different clusters and their stability by interpreting the interaction energy. A comparison with previous studies [1] on 3AP-water will be performed. Moreover, I would like to emphasise on the important role of the number of hydrogen bonds in the molecular clusters. In the last part of my presentation, I will provide IR spectra from the monomeric building blocks up to the tetramers and compare them with available experimental data. [2]



**Figure 1.** Structures andinteraction energies of 3AP-3AP dimer, and of clusters containing one or two water molecules

**References.**

[1] R. J. Lavrich, A-M. Kelterer, A. S. Khalil, J. Phys. Chem. A 121, 6646−6651 (2017)

[2] S. T. Mulla, C. I. Jose, J. Chem. SOC. Faraday Trans. I 82, 691-706 (1986)