

Dynamics of excited clusters of β -alanine in the gas phase

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Synopsis We present a theoretical study of excited clusters of β -alanine molecules in the gas phase: $(\beta\text{-ala})_n$, $n=2-5$. Classical molecular dynamics simulations performed for different internal excitation energies showed a thermal decomposition dependence with the cluster size. We also present an assessment study performed with different families of density functionals using the dimer, $(\beta\text{-ala})_2$ as a benchmark system. M06-2X provides the best agreement for the relative energies of 20 isomers in comparison with the reference values computed with the MP2 method. The stability and reactivity of several cluster sizes have been investigated with this functional in combination with the 6-311++G(d,p) basis set.

Ionization and excitation of biomolecules and clusters of biomolecules, induced with highly charged ions, is a widely employed technique to study the stability of these species at a molecular level. In these studies, modeling has become a fundamental tool for understanding the fragmentation dynamics [1,2]. We recently studied doubly-positively charged and excited monomers of β -alanine in the gas phase [3]. In a further step, we here present our recent investigations concerning the stability of clusters of this molecule in the gas phase. This is a more complicated system because it presents additional type of interactions between the molecules such as hydrogen bonds, van der Waals forces, etc. When amino acids are embedded in a cluster of molecules, a protective effect of the environment against fragmentation has been observed [4]. Thus, we evaluate which are the main effects behind this behavior.

We have first performed classical molecular dynamics (MD) simulations using the general amber force field including dimer, trimer, tetramer and pentamer clusters of β -alanine. Several trajectories for internal energies in the range $T=50-423\text{K}$ were carried out. With these simulations we studied the stability of the neutral clusters upon thermal excitations and we explore the potential energy surface, thus obtaining different structures.

In order to find a suitable computational tool for carrying out reliable electronic structure calculations for clusters of amino acids at a relatively low computational cost, an assessment based on density functional theory was performed. In our study we include different families of functionals, namely

B3LYP, B97D, M06, M06-2X and MPWB1K in combination with 6-311++G(d,p) basis set. The MP2 method was taken as a reference for the chosen model system $(\beta\text{-ala})_2$. The M06-2X method is shown to adequately reproduce the relative energies and geometries of 20 isomers of $(\beta\text{-ala})_2$.

Finally, we have used this level of theory to evaluate the relative stability of numerous isomers of different cluster sizes $(\beta\text{-ala})_n$, $n=2-5$. We have also studied ionization potentials and interaction energies. The possibility of inter- and intra-molecular reactions upon ionization and excitation of the clusters will be presented as well.

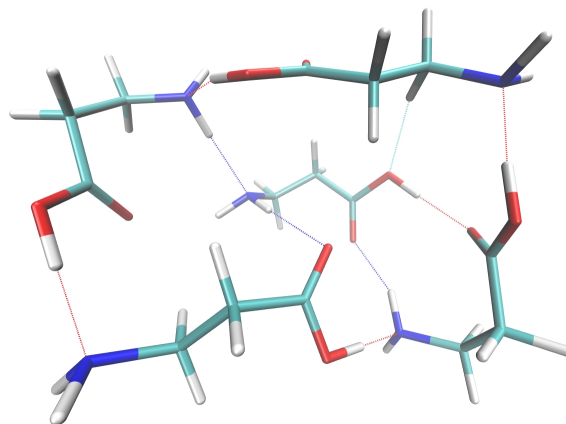


Figure 1. Stabilization of β -alanine clusters in the gas phase with intermolecular forces.

References

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