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A theoretical investigation of microhydration of amino acids

Catherine Michaux*, J Wouters, D Jacquemin, Eric A Perpète

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Water plays a role in stabilizing biomolecular structure and facilitating biological function. Water can generate small active clusters and macroscopic assemblies, that are able to transmit information on various scales [1]. Protonation and microhydration of proteins or DNA are of fundamental importance in biochemical processes such as proton transport, water-mediated catalysis, molecular recognition, protein folding, etc. The understanding of these hydration effects at the molecular level requires the characterization of the interactions between biomolecules and their environment. Due to its relevance in many fields, the microhydration process of nucleic acid bases or amino acids has received a widespread attention [2].

In this work, we first describe the microhydration of protonated amino acid (AA), and particularly of protonated glycine (GlyH+) [3][4], alanine (AlaH+) [5] and proline (ProH+) [6]. First a high-level theoretical method was setting up in order to compute the structures and properties of GlyH+-water complexes, Gly being the simplest AA and a suitable model for such a study. Then complexes with more than one water molecule as well as other amino acids (Ala and Pro) were investigated, to extend the validity domain of our computational procedure.

We then investigate a series of complexes made up of a deprotonated (anionic) AA and a single water molecule [7]. Such species have recently been identified with mass spectrometry, allowing meaningful comparisons between theoretical and experimental complexation energies. The selected systems are [Gly-H]-, [Ala-H]-, [Val-H]-, [Asp-H]-, [Gln-H]-, as well as the acetic acid as a model benchmark.

Unité de Chimie Physique Théorique et Structurale, Facultés Universitaires Notre-Dame de la Paix, rue de Bruxelles, 61, B-5000 Namur, Belgium

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