

Full protonation and also metal cation affinity of adenine in gas and solution phases; a theoretical study

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Adenine is a purine nucleobase. Purine is a heterocyclic aromatic organic compound that consists of two heterocyclic rings (pyrimidine and imidazole) fused together [1]. In this work, we report a theoretical study on protonation and metal cation affinity (Na^+ , K^+ , Mg^{2+} , Ca^{2+} , Fe^{2+} and Zn^{2+}) of adenine molecule at M06-D3 level of theory, with def2-TZVPP basis set using GAUSSIAN 09 program. The possibility of the protonation of different nitrogen atoms of the above molecule in both gas phase and aqueous solution was studied. The microprotonation constants for all different nitrogen atoms of adenine in solution was also computed. The complete protonation of this molecule was also investigated through our previously known methodology [2-4] and the most stable isomers for adenine H^+ , adenine H_2^+ , adenine H_3^+ , and adenine H_4^+ were determined in the gas phase. The possibility of the binding of adenine and its protonated form to metal ions through its different nitrogen atoms has been also studied (see Figure 1).

Keywords: Adenine, Proton affinity, Metal cation affinity, Gibbs free energy

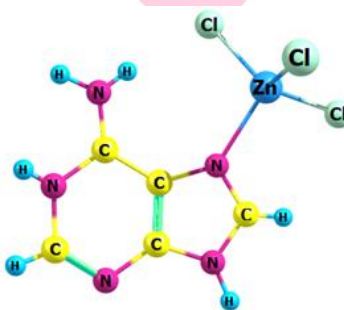


Figure 1. Optimized structure of a Zinc complex of the protonated adenine

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