Theoretical study of the deprotonation pathway of 6-OHDA in aqueous solution
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Abstract: 6-hydroxydopamine (6-OHDA) or 2,4,5-trihydroxyphenethylamine is a neurotoxic compound that used to induce the symptoms of Parkinson’s disease (PD) on experimental animal models. In aqueous solution, the functional groups of 6-OHDA, an amino (NH₂) and three hydroxy (OH) groups, can be deprotonated at different pH values. However, its deprotonation pathway has not been reported. Therefore, the structures of 6-OHDA involved in the deprotonation process and their interactions with its environment are still unclear. In this work, the optimized geometries, the proton affinity (PA), thermodynamics properties and LUMO distributions of the chemical species involved in the process of the 6-OHDA deprotonation in aqueous solution were studied by a means of the density functionals theory (DFT) at B3LYP/6-311++G** level of accuracy. These calculation data were used to establish and propose a plausible deprotonation pathway of 6-OHDA in aqueous solution. Additionally, the zwitterionic species, from the fully protonated 6-OHDA (6-OHDA⁺) to the neutral one, were revealed in this study. That is the proton is lost from the amino group of the fully protonated 6-OHDA.

Keywords: 6-OHDA; Deprotonation pathway; Parkinson’s disease; DFT