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STRUCTURES AND ISOMERIZATION OF NEUTRAL AND ZWITTERION SERINE-WATER CLUSTERS: COMPUTATIONAL STUDY

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Calculations are presented for the structure and the isomerization reaction of various conformers of the bare serine, neutral serine-$(H_2O)n$ and serine zwitterion-$(H_2O)n$ (n=1,2) clusters. The effects of binding water molecules on the relative stability and the isomerization processes are examined. Hydrogen bonding between serine and the water molecule(s) may significantly affect the relative stability of conformers of the neutral serine-$(H_2O)n$ (n=1,2) clusters. The sidechain (OH group) in serine is found to have a profound effect on the structure and isomerization of serine-$(H_2O)n$ (n=1,2) clusters. Conformers with the hydrogen bonding between water and the hydroxyl group of serine are predicted. A detailed analysis is presented of the isomerization (proton transfer) pathways between the neutral serine-$(H_2O)_2$ and serine zwitterion-$(H_2O)_2$ clusters by carrying out the intrinsic reaction coordinate analysis. At least two water molecules need to bind to produce the stable serine zwitterion-water cluster in the gas phase. The isomerization for the serine-$(H_2O)_2$ cluster proceeds by the concerted double and triple proton transfer mechanism occurring via the binding water molecules, or via the hydroxyl group.