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Effects of metal ion and solute conformation change on hydration of small amino acid

Natthiya Deeying, Kritsana Sagarik *

School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand

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Abstract

The effects of metal ion and solute conformation change on the structures, energetic and dynamics of water molecules in the first hydration shell of amino acid were studied, using three forms of alanine (Ala) and Li^+/Ala as model molecules. The theoretical investigations were started with construction of the test-particle model (T-model) potentials for all molecules involved and followed by molecular dynamics (MD) simulations of $[Ala]_{aq}$ and $[Li^+/Ala]_{aq}$ at 298 K. The MD results showed that the hydrogen bond (H-bond) networks of water at the functional groups of Ala are strengthened by the metal ion binding, whereas the rotation of the $N–C^{\alpha}$ bond from the angle $\phi = 0°$ to 180° brings about smaller effects which cannot be generalized. It was also shown that the dynamics of water molecule in the first hydration shell of amino acid could be estimated from the total–average potential energy landscapes and the water exchange diagrams. The MD results suggested inclusion of an additional dynamic step in the water exchange process, in which water molecule moves inside a channel within the first hydration shell of solute, before leaving the channel at some point. The theoretical results reported in the present work iterated the necessity to include explicit water molecules in the model calculations.

Keywords: Alanine; Lithium ion; Hydration; T-model; Residence time; Molecular dynamics simulations; Conformation