

STRUCTURES AND STABILITY OF MODEL SALT-BRIDGE INTERACTION IN AQUEOUS SOLUTION

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ABSTRACT: Structures and stability of model salt-bridge interaction in aqueous solution were investigated using complex formed from guanidinium (GN) and formate (FM) ions. The intermolecular potentials to describe the GN-H₂O, FM-H₂O and GN-FM interactions were constructed using the Test-particle model (T-model) and applied in Molecular Dynamics (MD) simulations of the aqueous solutions at 298 K. Although the charged hydrogen bonds (H-bonds) between GN and FM are quite strong, the hydration free-energy calculations showed the possibility for the solvent-separated structure in the aqueous solutions. The structures and energetic of the H-bond networks in the vicinities of the GN-FM complex were visualized and discussed based on probability distribution (PD) maps and the average potential energy landscapes.

KEYWORDS: T-model, guanidinium, formate, salt bridge, aqueous solution