SOLVATION OF Zn(II) IN HYDROTERMAL SOLUTION BASED ON CLASSICAL MOLECULAR DYNAMICS SIMULATIONS

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ABSTRACT

This study aims to investigate the structure and dynamics of the solvation properties of Zn(II) ions in hydrothermal solutions through classical molecular dynamics simulations.
The research steps include a) selection of good base sets; b) preparation of new 2-body and 3-body potentials for Zn2+-H2O and H2O-Zn2+-H2O interactions, c) classical MD simulations at various temperatures (25, 50, 75, 100, 150, 200, 250, 300, and 350 oC), which takes into account the effects of two bodies (2-body MM) and three bodies (2-body MM + 3-body). The simulation system consists of a Zn2+ ion) and 499 water molecules, and d) trajectory analysis of the simulation results to determine the structural properties and solvation dynamics of the ions in the hydrothermal solution.
The results showed that in the hydration structure of Zn2+, the distance of the Zn2+-H2O ion in the first hydration shell was affected by the simulation temperature although it was very small while the number of water molecules coordinated to the central ion Zn2+ at T = 25, 50, 75 and 100 ^{o}C was 6 but the number of it decreases to only 4 H2O molecules at T = 150, 200, 300 and 350 ^{o}C. The hydration structure of the Zn2+ ion changes from a distorted octahedral to a distorted tetrahedral. The effect of temperature on the hydration dynamics of the Zn2+ ion is shown by the exchange of H2O ligands between the first and second hydration shells at temperatures of 150, 200, 250, 300, and 350 ^{o}C while at temperatures of 25, 50, 75, and 100 ^{o}C the ligand exchange was not observed. . The hydration stability of the skin first appears to be affected by increasing temperature.

Kata Kunci: *solvation, hydrothermal, Zn(II), classical molelecular dynamics simulations*