Preferential Solvation of Zr(IV) and Zn(II) Ions in 18.6% Ammonia Solution Based on the Quantum Mechanics / Molecular Mechanics (QM /MM) Molecular Dynamics Simulation

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ABSTRACT

Abstract

This study aims to investigate the preferential solvation of Zr(IV) and Zn II) ions in 18.6% ammonia solution through quantum mechanics / molecular mechanics (MD QM / MM) molecular dynamics simulations.
The research steps include a) selecting a good basis sets; b) new 2-body and 3-body potentials for the interaction of ions-H_2O and ion-NH_3 as well as H_2O-ion-H_2O, NH_3-ion-NH_3 and H_2O-ion-NH_3; c) classic MD simulation and MD QM/MM. In molecular dynamics simulation is carried out by taking into account the influence of two bodies (MM 2-body), three bodies (MM 2-body + 3-body) and multiple bodies (QM/MM). The three simulation systems consist of an ion, with 499 water molecules, 215 ammonia molecules and a 18.6% ammonia solution; and d) trajectory analysis of the simulation results to determine the structural properties and prefer the ions (Zr^{4+} and Zn^{2+}) to ammonia ligands in 18.6% ammonia solutions.
The results showed that the solvation structure of $[Zn(NH_3)_4]^{2+}$ was observed in a 18.6% ammonia and Zn^{2+} solutions more easily coordinated with ammonia ligands than H_2O ligands. Likewise, because the ratio of the number of ligands NH_3 and H_2O in the complex $[Zr(NH_3)_3\ (H_2O)_5]^{4+}$ in the first shell is 3/5 (0.60) while in the mixed ammonia-water system it is 92/407 (0.22). The mole fraction of ammonia (local composition) is greater than the mole fraction of water in the first shell compared to the mole fraction in the bulk phase so that Zr^{4+} and Zn^{2+} ions are more easily (preferentially) coordinated by ammonia than water ligands and preferentially according to Lewis acid-base interaction concept.

Kata Kunci: *preferential solvation, QM/MM simulations, 18,6% ammonia solutions*