STRUCTURE AND DYNAMICS OF GROUP IIB HYDRATION IONS USING MOLECULAR MECHANICS SIMULATION DYNAMICS

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ABSTRACT

The metabolic processes that reside in the body of a living being, always involve various solvents both water and non water. The human body mostly (more than 80%) consists of liquids, so the process of metabolism in the human body involves the interaction between solvents and solutes both in the form of ions and their compounds. The interaction between solvent and solute is known as solvation. While the interaction of solutes with water known as hydration. Group IIB is a class of transition metal containing elements of Cd, Zn, and Hg. The element to be observed for the hydration of water is limited to the Zn and Cd elements.
Zn and Cd solvation was observed by simulating the molecular dynamics of molecular mechanics. The basic set used is lanl2dz for Zn and Cd atoms, while for water molecules used DZP dynamic base association. The simulation is done by using potential pair and potential 3 body. Each Zn and Cd simulation is done by mixing 1 Cd and Zn atoms mixed with 499 H_2O molecules. The simulation result in the form of trajectory data is further processed to know the structure and dynamics
The result of RDF analysis shows that the distance of Zn atom and the average O (water) atom is 2.18 A, while the average distance of Cd atom with 2.27 A. Based on CND analysis it is known that the coordination number of Cd and Zn solvation in water is equal 6. There is known that both solvations form the octahedral molecular structure. The residence time of ligand (water) in Zn based on the molecular dynamics analysis shows that the solvation of Zn with water is more unstable than the solvation of Cd^{2+} ions.

Kata Kunci: *Cd ions, Zn ion, hydration, and DMMM*