STRUCTURE AND DYNAMICS OF ION Hg2+ IN WATER, LIQUID AMMONIA AND AMMONIA-WATER MIXED BASED ON SIMULATION STUDY OF DYNAMICS OF QUANTUM MECHANICA / MOLECUL MECHANICA MOLEKUL (MK / MM)

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ABSTRACT

The metabolic process that is in the body of living things, always involves various solvents, both water and non-water. The human body mostly (more than 80%) consists of liquid, so that the metabolic processes in the human body involve the interaction between solvents and solutes in both ionic and compounds. The interaction between solvents and solutes is known as hydration. While the interaction of dissolved substances with water is known as hydration. Mercury is a transition metal element located in group IIB period 6. Metal mercury is a toxic metal, can cause poisoning. Chronic poisoning by mercury can occur due to skin contact, food, drink and breathing. Chronic toxicity in the form of disorders of the digestive system and nervous system, impaired lens of the eye and can cause damage to the fetal brain resulting in disability in babies born.

Solvation of mercury ions is observed by conducting molecular dynamics simulations of molecular mechanics. The base set used is DEF2-ECP for Hg atoms, while for water and ammonia molecules a dunning DZP base is used. Simulation is done using potential partners and potential 3 bodies. The simulation is done by mixing 1 Hg2 + ion mixed with 499 H2O molecules and the second by mixing 1 Hg2 + ion mixed with 215 NH3 molecules. The simulation results in the form of trajectory data are further processed to find out the structure and dynamics.

Based on RDF analysis shows that the average Hg and O (water) atoms are 2.22 A while the Hg and N (ammonia) atoms are on average 2.35 A. Based on CND analysis it is known that the coordination number of Hg hydration in water equal to 6 water molecules while the coordination numbers of Hg in ammonia are as much. Thus it is known that the hydration of Hg ions in water forms the structure of the distorted octahedral molecule and the solvation of Hn ions in ammonia breaks down the tetrahedral structure. Graph analysis of ligand displacement shows that the ammonia ligand residence time is longer than water

Kata Kunci: *solvation, Mercury, QM/MM MD*