Widhiyanto, H., 2006, Monte Carlo Simulation to obtain solvation structure of Ni(II) in concentrated ammonia using two-body potential. The script guided by Drs. Faidur Rochman, MS. and Drs. Imam Siswanto, M.Si., Department of Chemistry, Mathematic and Science Faculty, Airlangga University, Surabaya

ABSTRACT

Monte Carlo simulation for Ni^{2+} in concentrated ammonia solution using two body potential was carried out in order to study preferential solvation. Interaction potential of $H_2O - H_2O$, $NH_3 - NH_3$, $H_2O - NH_3$, $Ni^{2+} - H_2O$, $Ni^{2+} - NH_3$ adopted from literatures used for simulation input. Simulation system consist of 1 ion Ni^{2+}, 210 H_2O and NH_3 molecules whereas each quantity have been adjusted by the concentrations. The simulation is running at 293,15 K in order to keep the system in liquid state. The results show that first solvation shell of Ni^{2+} consist of 6 NH_3 molecules at 49,76% and 59,72% ammonia solution. Whereas at 69,67% and 79,62% ammonia solvation are 8 NH_3 molecules. The amount of H_2O and NH_3 molecules in the second solvation shell of Ni^{2+} ion are 3 and 8 at 49,62%; 1 and 19 at 59,72% ; 2 and 19 at 69,67%; 0 and 21 at 79,62% respectively. Distribution data of angle, radial and solvation number indicate two geometry structure that are triangle antipiramidal and quadrangle antipiramidal.

Keywords : *Monte Carlo simulation, Two-body potential, Preferential solvation.*