Structure and dynamics of Cd2+ in liquid ammonia: Insight from An ab initio QM/MM MD Simulations

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ABSTRACT

Abstract
The structure and dynamics of solution Cd(II) in liquid ammonia environment have been investigated by means of an ab initio QM/MM molecular dynamics (MD) simulations at the Hartree-Fock level. In this method, the region comprises Cd(II) ion and ligand in the first solvation shell were investigated by ab initio quantum mechanical Born-Oppenheimer while the rest of the system are described as classical 2-body and 2-body + 3-body potential. Structural properties were indicated by some parameters, namely the coordination number distribution (CND), radial distribution function (RDF), and angle distribution function (ADF), while the dynamical properties were characterized by the mean ligand residence time (MRT) and ligand exchange occurence. The Solvation number of 6 was found through the QM/MM methods with the modified SBKJC VDZ ECP basis set for Cd(II) ion and DZP for N and H, in contrast to 10 obtained through 2-body potential simulation. No ligand exchanges were indicated between the first and second shell. The mean ligand residence time in the second solvation shell is 4.419 ps.

Kata Kunci: *ab initio QM/MM MD method, 2-body + 3-body potential, Cd(II) ion, liquid ammonia, solvation*