INTISARI

KAJIAN STRUKTUR DAN DINAMIKA SOLVASI BERILIUM(II) DALAM AMMONIA CAIR MENGGUNAKAN SIMULASI DINAMIKA MOLEKULAR *QMCF* (*QUANTUM MECHANICAL CHARGE FIELD)*

Oleh

Priyagung Dhemi Widiakongko
14/373329/PPA/04791

Solvasi ion Be^{2+} dalam amoniak cair telah dipelajari menggunakan metode simulasi dinamika molekular QMCF (*quantum mechanical charge field*). Protokol simulasi yang dijalankan adalah sistem ion Be^{2+} di dalam 957 molekul NH_3 dengan model fleksibel NH_3. Temperatur selama simulasi dijaga tetap dengan sistem thermostat Berendsen.

Hasil dari simulasi dinamika molekular selama 8 ps adalah ion Be^{2+} disolvasi oleh 4 molekul NH_3 secara tetrahedral dengan sudut 107 ^{o} pada jarak 1,745 Å dalam kulit solvasi pertama. Tidak ada usaha pertukaran ligan teramati selama waktu simulasi 8 ps. Hal ini menunjukkan sistem solvasi ion Be^{2+} dengan NH_3 merupakan sistem yang stabil. Kulit solvasi kedua menunjukkan struktur yang lebih labil dengan banyak pertukaran ligan yang sukses. Hasil simulasi memberikan data yang hampir dengan hasil eksperimen.

Kata kunci: Be^{2+}, solvasi, ammonia cair, *quantum mechanical charge field* (QMCF), simulasi dinamika molekular

ABSTRACT

THE STUDY OF STRUCTURE AND SOLVATION DYNAMICS OF BERYLLIUM (II) ION IN LIQUID AMMONIA USING QUANTUM MECHANICAL CHARGE FIELD (QMCF) MOLECULAR DYNAMICS SIMULATION

by

Priyagung Dhemi Widiakongko
14/373329/PPA/04791

The solvation of Be^{2+} ion in liquid ammonia has been investigated using an ab initio Quantum Mechanical Charge Field Molecular Dynamics (QMCF – MD). The simulation protocol has been set by performing one Be^{2+} ion in 957 ammonia molecule with flexible model of ammonia. The simulation temperature was kept constant during the work by Berendsen Thermostat system.

The result of molecular dynamics simulation conducted that within 8 ps time of simulation, the Be^{2+} ion is tetrahedrally coordinated by four ammonia molecules at a distance of 1,745 Å in the first solvation shell. The N-Be-N angle obtained is 170^{o}. The second solvation shell shows a labile structure with large number of successful ligand exchange. The simulation results has a good agreement with the experiments.

Keywords: Be^{2+} ion, solvation, liquid ammonia, quantum mechanical charge field (QMCF), molecular dynamics simulation