KAJIAN STRUKTUR DAN DINAMIKA HIDRASI ION Mg^{2+} DALAM AIR MENGGUNAKAN SIMULASI DINAMIKA MOLEKUL MEKANIKA MOLEKUL 2-BADAN

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INTISARI

Sifat struktur dan dinamika hidrasi ion Mg^{2+} dalam pelarut air telah dipelajari menggunakan simulasi dinamika molekul MM 2-badan. Penelitian bertujuan untuk membuat potensial Lennard-Jones yang akurat pada interaksi ion Mg^{2+} dan model air SPC/E dan mempelajari struktur dan dinamika hidrasi ion Mg^{2+} dalam air. Metode simulasi yang digunakan ditentukan berdasarkan nilai BSSE dan persamaan potensial 2-badan yang akurat. Jarak ion Mg^{2+} dan ligan air diperoleh dengan simulasi dinamika molekul dengan memperhitungkan pengaruh 2-badan. Simulasi dinamika molekul MM 2-badan dilakukan pada sistem yang terdiri dari 2000 molekul air dan 1 ion Mg^{2+}. Sifat struktur dan dinamika hidrasi ion Mg^{2+} dikarakterisasi menggunakan fungsi distribusi radial (RDF), fungsi distribusi angular (ADF), waktu tinggal ligan rata-rata (MRT) dan bilangan koordinasi (CND).

Analisis data menunjukkan kulit hidrasi pertama bersifat fleksibel dengan variasi jumlah ligan air 7 dan 8. Probabilitas bilangan koordinasi tertinggi dalam simulasi membentuk dua geometri yang stabil yaitu $[Mg(H_2O)_7]^{2+}$ dan kompleks $[Mg(H_2O)_8]^{2+}$ dengan geometri *monocapped trigonal antiprism* (MTAP) dan *square antiprism* (SA). Sudut ikatan pada jarak 2,1 Å diperoleh sebesar 75,51^o dan 139,50^o. Kulit hidrasi kedua bersifat lebih labil dibuktikan dengan variasi jumlah ligan yang cukup banyak dan rata-rata waktu tinggal ligan yang sangat singkat. Vibrasi ulur ikatan Mg-O diperoleh pada panjang gelombang 480,04 cm^{-1} dengan koefisien gaya sebesar 130,98 Nm^{-1}.

Kata kunci: 2-badan, dinamika molekul, hidrasi, Mg^{2+}

HYDRATION STRUCTURES AND DYNAMICS STUDY OF Mg^{2+} ION IN WATER USING 2-BODY MOLECULAR MECHANICS MOLECULAR DYNAMIC SIMULATION

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ABSTRACT

Structure and dynamics properties of Mg^{2+} ion in aqueous water were investigated using classical molecular dynamics simulations based on an accurate two-body molecular mechanics (MM) potential. This study aimed to develop a reliable Lennard–Jones potential for the interaction between the Mg^{2+} ion and water molecules described by the SPC/E model, and to elucidate the hydration structure and dynamics of Mg^{2+} in water. The simulation protocol and potential parameters were established based on basis set superposition error (BSSE) considerations and a physically consistent two-body interaction potential. The Mg^{2+}–water distances were obtained from molecular dynamics simulations explicitly accounting for two-body effects. The simulations were performed on a system consisting of one Mg^{2+} ion solvated by 2000 water molecules. The structural and dynamical features of Mg^{2+} hydration were characterized using the radial distribution function (RDF), angular distribution function (ADF), mean residence time (MRT) of water ligands, and coordination number distribution (CND).

The results indicate that the first hydration shell of Mg^{2+} is flexible, with coordination numbers fluctuating between 7 and 8. The highest coordination number probabilities correspond to two stable hydrated complexes, $[Mg(H_2O)_7]^{2+}$ and $[Mg(H_2O)_8]^{2+}$, adopting monocapped trigonal antiprism (MTAP) and square antiprism (SA) geometries, respectively. The characteristic O–Mg–O bond angles at a Mg–O distance of 2.1 Å were found to be 75.51° and 139.50°. In contrast, the second hydration shell exhibits a more labile nature, as evidenced by a broader coordination number distribution and significantly shorter ligand residence times. The Mg–O stretching vibration was identified at a wavenumber of 480.04 cm^{-1}, corresponding to a force constant of 130.98 N m^{-1}. These findings provide a comprehensive description of the hydration structure and dynamics of Mg^{2+} in water and demonstrate the reliability of the developed two-body potential for modeling ion–water interactions.

Keywords: 2-body, hydration, Mg^{2+}, molecular dynamics.