INTISARI

KAJIAN TEORITIS SIFAT STRUKTUR DAN DINAMIKA ION Sc^+ *SINGLET* (^1D) DAN *TRIPLET* (^3D) DALAM AIR, AMONIAK CAIR, DAN CAMPURAN AMONIAK-AIR MENGGUNAKAN SIMULASI DINAMIKA MOLEKULER *AB INITIO* MEKANIKA KUANTUM/MEKANIKA MOLEKULER

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Sifat struktur dan dinamika solvasi ion Sc^+ *singlet* (^1D) dan *triplet* (^3D) dalam air, amoniak cair, dan campuran amoniak-air telah dipelajari melalui simulasi dinamika molekuler mekanika kuantum/mekanika molekuler (DM MK/MM). Himpunan basis LANL2DZ ECP digunakan untuk ion Sc^+ *singlet* (^1D) dan ion *triplet* (^3D), sedangkan DZP-DUNNING untuk atom N, O, dan H.

Simulasi DM MK/MM ion Sc^+ *singlet* (^1D) dan *triplet* (^3D) dalam air dilakukan dengan kondisi 1 ion Sc^+ *singlet* (^1D) dan *triplet* (^3D) dalam 499 molekul air, dan suhu 298,16 K, sesuai dengan densitas air pada suhu tersebut 0,991 g cm^{-3}. Simulasi DM MK/MM dalam amoniak cair dilakukan dengan kondisi 1 ion dalam 215 amoniak, suhu 235,26 K, sesuai dengan densitas amoniak cair pada suhu tersebut 0,690 g cm^{-3}. Simulasi DM MK/MM dalam campuran amoniak-air dilakukan dengan kondisi 1 ion dalam campuran 92 molekul amoniak dan 407 molekul air, suhu 298,16 K, sesuai dengan densitas campuran amoniak-air pada suhu tersebut 0,927 g cm^{-3} dan konsentrasi 18,6 % amoniak.

Simulasi DM MK/MM ion Sc^+ *singlet* (^1D) dan *triplet* (^3D) dalam air, amoniak cair dan campuran amoniak-air dilakukan selama sekitar 25 ps. Struktur solvasi pertama dalam air terlihat ion Sc^+ *singlet* (^1D) mengikat 3 molekul air, sedangkan ion Sc^+ *triplet* (^3D) 2 molekul air. Kedua struktur solvasi kulit pertama tersebut bersifat rigid. Struktur solvasi kulit pertama ion Sc^+ *singlet* (^1D) dalam amoniak cair mengikat 3 molekul amoniak, sedangkan ion Sc^+ *triplet* (^3D) 2 molekul amoniak. Kedua struktur inipun bersifat rigid. Struktur solvasi kulit pertama ion Sc^+ *singlet* (^1D) dalam campuran amoniak-air terlihat membentuk kompleks $[Sc(NH_3)_2(H_2O)_2]^+$ dan $[Sc(NH_3)_2(H_2O)_3]^+$, sedangkan ion Sc^+ *triplet* (^3D) dalam campuran amoniak-air membentuk struktur kompleks $[Sc(NH_3)_2(H_2O)]^+$ dan $[Sc(NH_3)_2(H_2O)_2]^+$. Struktur solvasi ion Sc^+ *singlet* (^1D) dan Sc^+ *triplet* (^3D) dengan amoniak bersifat rigid, sedangkan ion Sc^+ *singlet* (^1D) dan Sc^+ *triplet* (^3D) dengan air bersifat dinamis, karena selama simulasi terjadi pertukaran ligan.

Kata kunci: simulasi DM MK/MM, Sc^+ *singlet* (^1D), Sc^+ *triplet* (^3D), air, amoniak

ABSTRACT

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THEORETICAL STUDY OF STRUCTURAL AND DYNAMICAL PROPERTIES OF SINGLET (^{1}D) Sc^+ AND TRIPLET (^{3}D) IONS IN WATER, LIQUID AMMONIA, AND AMMONIA-WATER MIXTURE USING MOLECULAR DYNAMICS SIMULATION OF *AB INITIO* QUANTUM MECHANICS/MOLECULAR MECHANICS

Structural and dynamical solvation properties of Sc^+ *singlet* (^{1}D) and Sc^+ *triplet* (^{3}D) ions in water, liquid ammonia and ammonia-water mixture have been studied using quantum mechanics/molecular mechanics molecular dynamics (QM/MM MD) simulation. The basis set Lanl2dz ecp was used for Sc^+ *singlet* (^{1}D) and Sc^+ *triplet* (^{3}D) ions, while DZP (Dunning) for N, O, and H atoms

QM/MM MD simulation ion in water was conducted under one ion in 499 water molecule, at temperature 298.16 K, in accordance with density of water 0.9907 g cm^{-3}. QM/MM MD simulation in liquid ammonia was performed under one ion in 215 ammonia at temperature 235.26 K, in accordance with the density of liquid ammonia 0.690 g cm^{-3}. QM/MM MD simulation in ammonia-water mixture was conducted under one ion in mixture of 92 ammonia and 407 water molecules at temperature of 298.16 K, in accordance with the density of ammonia-water mixture 0.9270 g cm^{-3} and a concentration of 18.6% ammonia

QM/MM MD simulation of Sc^+ singlet (^{1}D) and Sc^+ triplet (^{3}D) ions in water, liquid ammonia and ammonia-water mixture are performed about 25 ps obtaining the following results. First solvation structures of ion in water show Sc^+ singlet (^{1}D) binds 3 molecules of water, meanwhile the Sc^+ triplet (^{3}D) two water molecules. Both structures of the first solvation shells are rigids. The first solvation shell structures of ion in liquid ammonia show Sc^+ singlet (^{1}D) binds 3 molecules of ammonia, meanwhile Sc^+ triplet (^{3}D) two ammonia molecules. Both structures are also rigids. The first solvation shell structure of Sc^+ singlet (^{1}D) ion in ammonia-water mixture is composed $[Sc(NH_3)_2(H_2O)_2]^+$ and $[Sc(NH_3)_2(H_2O)_3]^+$ complex, meanwhile Sc^+ triplet (^{3}D) ion in ammonia-water mixture shows $[Sc(NH_3)_2(H_2O)]^+$ and $[Sc(NH_3)_2(H_2O)_2]^+$ complex structure. Solvation structures of Sc^+ singlet (^{1}D) and Sc^+ triplet (^{3}D) ions with ammonia are rigid, meanwhile Sc^+ singlet (^{1}D) and Sc^+ triplet (^{3}D) ions with water are dynamic, due to the occurrence of ligand exchanges during simulation time.

Keywords: QM/MM MD, Sc^+ singlet (^{1}D), Sc^+ triplet (^{3}D), water, ammonia