KAJIAN STRUKTUR DAN DINAMIKA SOLVASI ION Ac^{3+} DALAM AIR MENGGUNAKAN SIMULASI DINAMIKA MOLEKUL MP2-DKH2/MM

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INTISARI

Kajian struktur dan dinamika solvasi ion Ac^{3+} dalam air berdasarkan simulasi dinamika molekuler MP2-DKH2/MM telah dilakukan. Tujuan penelitian ini adalah melakukan kajian teoritis pembentukan kompleks $[Ac(H_2O)_n]^{3+}$ dan kestabilannya dalam larutan berair serta mempelajari sifat struktur dan dinamika solvasi ion Ac^{3+} dalam air secara komputasi. Analisis trajektori dilakukan untuk mempelajari sifat struktur dan dinamika solvasi ion Ac^{3+} dalam air yang meliputi fungsi distribusi radial (RDF), distribusi bilangan koordinasi (CND), fungsi distribusi sudut (ADF), waktu tinggal rata-rata ligan (MRT), vibrasi ulur Ac^{3+}-O, dan *local density corrected three-body distribution functions*.

Simulasi dinamika molekul MP2-DKH2/MM menggunakan metode *ab initio* MP2. Himpunan basis relativistik SARC-DKH-TZVP diberlakukan untuk ion Ac^{3+} dan himpunan basis 6-31G* untuk air. Koreksi efek relativistik untuk ion Ac^{3+} dihitung menggunakan metode DKH2. Ekuilibrasi sistem dilakukan selama 5 ps yang kemudian dilanjutkan dengan proses *sampling* data selama 100 ps. Hasil penelitian menunjukkan bahwa kulit solvasi pertama bersifat *rigid*/kaku yang membentuk kompleks stabil oktahidrat ($[Ac(H_2O)_8]^{3+}$) yang tertata dalam geometri *Square Antiprism* (SA) dan nonahidrat ($[Ac(H_2O)_9]^{3+}$) yang tertata pada geometri *Gyro-elongated Square Antiprism* (GySA) di mana terdapat 8 hingga 9 molekul H_2O. Sudut ikatan yang diperoleh sebesar 72,5º dan 138,5º pada jarak 2,68 Å. Kulit solvasi kedua dan ketiga bersifat dinamis dan memiliki fleksibilitas tinggi dibuktikan dengan waktu tinggal ligannya yang cukup singkat yaitu berturut-turut sebesar 6,46 ps dan 2,67 ps.

Kata kunci : Ac^{3+}, air, MP2-DKH2/MM, relativistik, solvasi

STRUCTURE AND DYNAMICS OF SOLVATED Ac^{3+} ION IN WATER: A MP2-DKH2/MM MOLECULAR DYNAMICS SIMULATION STUDY

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ABSTRACT

A study of solvation structure and dynamics of Ac^{3+} ion in water based on MP2-DKH2/MM molecular dynamics simulation has been carried out. The aims of this research are to conduct a theoretical study of formation $[Ac(H_2O)_n]^{3+}$ complex and its stability in aqueous solution and to study the structural properties and dynamics of solvation of the Ac^{3+} ion in water using computational method. Trajectory analysis was carried out to study the structural properties and dynamics of solvation of Ac^{3+} ions in water which includes Radial Distribution Function (RDF), Coordination Number Distribution (CND), Angular Distribution Function (ADF), Mean Residence Time (MRT), stretching vibration of Ac^{3+}-O, and local density corrected three-body distribution functions.

MP2-DKH2/MM molecular dynamics simulations used the MP2 ab initio method. The SARC-DKH-TZVP relativistic basis set was applied to Ac^{3+} ion and 6-31G* basis set was applied to water molecules. The correction of relativistic effect for Ac^{3+} ion was calculated using the DKH2 method. System equilibration was carried out for 5 ps which was then continued with a sampling process for 100 ps. The result of this research shows that the first solvation shell is rigid which forms a stable complex of octahydrate actinium complex ($[Ac(H_2O)]^{3+}$) which is arranged in Square Antiprism (SA) geometry and nonahydrate actinium complex ($[Ac(H_2O)_9]^{3+}$) which is arranged in Gyro-elongated Square Antiprism (GySA) geometry where there are 8 until 9 H_2O molecules. The obtained bond angles were 72.5º and 138.5º at a distance of 2.68 Å. The second and third solvation shells are dynamic and have high flexibility as evidenced by their relatively short ligand residence times, namely 6.46 ps and 2.67 ps respectively.

Keywords: Ac^{3+}, MP2-DKH2/MM, relativistic, solvation, water