MOLECULAR DYNAMICS SIMULATIONS OF RU (II) IN WATER INCLUDING THREE-BODY CORRECTION

Kusumawardani, C, Armunanto, Ria, Suwardi, and Pranowo, H.D.

In order to describe the cobalt-water interaction correctly, a new ab ibitio potential was developed consisting of pair interaction terms as well as three-body contributions. Within this approach, it was possible to correct for the well-known failures of pair potentials in describing solvation phenomena of such ions. A first-shell coordination number of 6 in agreement with experimental data were obtained from Molecular Dynamics simulations of a single ruthenium (II) ion in water. The structure of hydrated ion is discussed in terms of radial density functions and coordination number, energy and angular distributions.

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