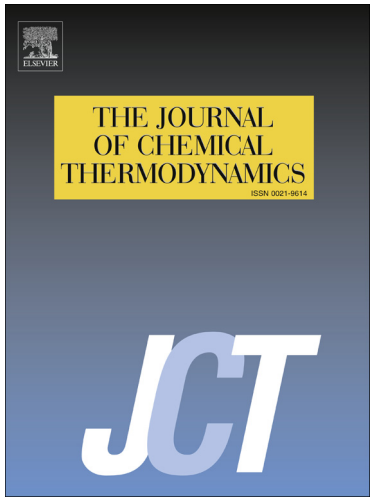

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The organisation of water around creatine and creatinine molecules

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Abstract

The densities and viscosities of creatine and creatinine in aqueous solutions were measured in the temperature range from T = (293.15 to 313.15) K. The theoretical aspects, molecular dynamics (MD) simulations and radial distribution functions (RDFs), have been applied, in order to understand the nature of interactions and water organisation in the studied systems. From the obtained values of the apparent molar volumes at infinite dilution (V_ϕ^o), the excess partial molar volumes of water ($V_{m_2}^E$), the Heppler's coefficients, viscosity *B*-coefficients and hydration numbers, a structure making/breaking properties creatine and creatinine in aqueous solutions were investigated. Influence of temperature on the conversion rate of creatine to creatinine has been linked with their solvation properties. Taste behaviour of creatine and creatinine have been investigated, also.

Keywords: creatine; creatinine; volumetric properties; viscosity; MD simulation; hydration number; taste.

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