

Temperature dependence studies and microscopic protonation constants of L-alanine and β -alanine in acetonitrile – water mixtures

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Abstract. L-alanine and β -alanine are important biological molecules and have zwitterion structure. In this study, L-alanine and β -alanine's microscopic protonation constants and thermodynamic parameters (enthalpy, entropy, and free energy changes) for the proton–ligand systems of L-alanine methyl ester, β -alanine and β -alanine methyl ester have been determined at 5; 20; 35 °C, in ACN-water (25% ACN and 50% ACN (v/v)) mixtures at constant ionic strength of 0.1000 mol L⁻¹ NaClO₄ by potentiometric method. The results shown that, L-alanine and β -alanine's microscopic protonation constants generally tend to decrease with temperature rise and their protonation reactions in ACN-water mixtures generally favor enthalpy-driven.

Keywords: L-alanine, β -alanine; microscopic protonation constants; thermodynamics parameters.

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