

Thermodynamics of transfer of atomic and molecular species into binary solvents

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Abstract

A method was suggested for separation of the Gibbs energy of transfer of atomic, molecular species from a solvent Solv1 into a binary solvent (Solv1 + Solv2) into the contribution from solvation of the reaction centers and that from nonspecific interactions, solvent reorganization, and cavity formation. The relationship for calculating the former contribution can be used for thermodynamically adequate comparative estimation of the stability of complex species in solution.

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