Russian Journal of Physical Chemistry A 2000 vol.74 N10, pages 1592-1595

Solvent effects on the conformational equilibrium parameters of heterocyclic compounds

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Abstract

The dependences of the thermodynamic parameters of equilibria (Gibbs energies ΔG and enthalpies ΔH) on the dielectric properties of solvents (carbon disulfide, toluene, chloroform, methylene chloride, acetone, and acetonitrile) were analyzed for six types of heterocyclic systems, for which various types of conformational equilibria were observed. The obtained relations between the slopes of the linear dependences of the enthalpies and Gibbs energies of conformational equilibria on medium polarity and the difference of the squares of the dipole moments of the conformers showed that the model of dipole-dipole conformer-medium interactions was incomplete.