Is the hydration number of a non-electrolyte additive with length and constituents of the solute molecule?

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Streszczenie

Sound velocity and density were measured at 298.15K in a number of very diluted aqueous solutions of simple non-electrolytes: alcohols, amines and acids. From these data the adiabatic compressibilities were calculated, and further the hydration numbers of solutes using the Passynski formula. It was found that all the homologous series under investigation exhibit linear concentration dependence of compressibility – and, consequently, that of the hydration numbers – up to concentrations of ca. 0.01 mole fraction or more. The slopes of these dependences are decreasing and nh's are increasing with the molecular mass of the solute. This observation suggests that hydration numbers nh are additive with the constituents of the molecule. Moreover, it would also imply the conclusion that local loss in compressibility of water solvent caused by hydration is very short in distance. To test the above assumption the hydration numbers were calculated using partial hydration numbers (i.e. those assigned to specific functional groups of the solute
molecules), the latter are fitted parameters. The obtained values of partial nh's are ca. 0.5 for –OH group, ca. 1.15 for –COOH and –NH2 and from 0.5 to ca. 1.3 for hydrocarbon elements of the hydrophobic chain (–CH2– and –CH3 groups). The
obtained total nh's are surprisingly close to the experimentally obtained hydration numbers. There are, however, systems where differences between calculated and experimental nh's are exceeding the experimental uncertainty; they are amino
acids and diols, particularly α, ω-diols. The reasons are, most possibly, interaction of the hydration shells of the hydroxyl groups in the latter case and formation of two charged sites in the zwitterionic form of the former ones.