SURFACE TENSION OF ACETONITRILE AND AQUEOUS SOLUTIONS

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We present results for the surface tension of acetonitrile at different temperatures. Molecular dynamics simulations in a canonical ensemble were performed. United-atom and all-atom representations for acetonitrile were used for reaching our purpose. The surface tension for acetonitrile was estimated over a wide range of temperature [300--450]K. The capabilities of rigid and flexible models were explored. The best performance was obtained from a rigid three-site model by using virtual sites to keep rigid the molecule. The obtained results were compared with the experimental ones which are available only at low temperatures, from this comparison an excellent agreement was found. The liquid-vapor equilibrium densities were also estimated and our results were compared with data derived from an empirical equation. A good agreement was obtained after the comparison. The binary mixture water-acetonitrile at different concentrations was also analyzed. The surface tension for these mixtures was estimated, varying the acetonitrile concentration at different temperatures [298 and 340] K. This property shows unstable configurations into the concentration region χ=[0.125--0.50], around T=298 K. Finally, at a higher temperature T=340K such configurations vanish.