Effects of osmolytes on the hydrogen bonding structure and dynamics in aqueous N-methylacetamide solution

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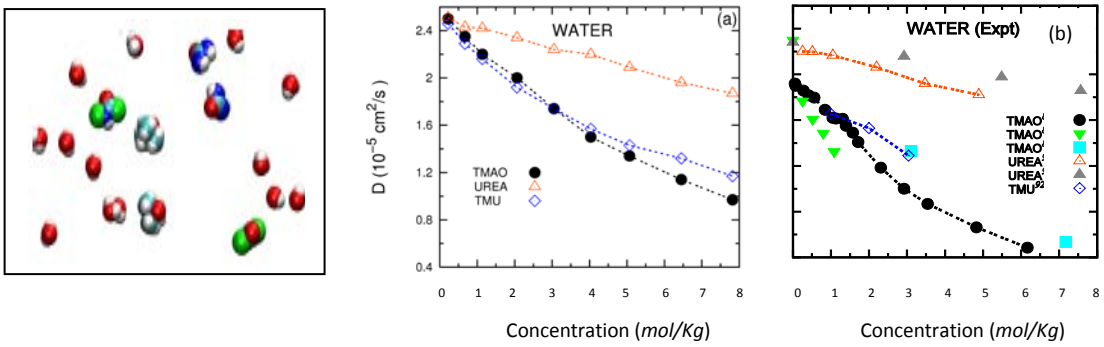
The effects of trimethylamine-N-oxide (TMAO), urea and tetramethyl urea (TMU) on the hydrogen bonding structure and dynamics of aqueous solution of N-methylacetamide are investigated by classical molecular dynamics simulations. The alteration of water structure and interaction between water and NMA in presence of these osmolytes are calculated by different site-site radial distribution functions and average interaction energies between these species in the solution. It is observed that the number of four hydrogen bonded water molecules in the solution decreases significantly in case of TMAO than the urea and TMU. The lifetime and structural relaxation time of water-water and NMA-water hydrogen bonds shows a strong increase with addition of TMAO and TMU in the solution, whereas the change is nominal in case of urea solution. It is also found that the translational and rotational dynamics of water [1-3] and NMA slowdown with increasing the concentration of osmolytes. The slower dynamics of water and NMA is more pronounced in case of TMAO and TMU solution, as these osmolytes strengthen the average hydrogen bond energies between water-water and NMA-water, whereas urea has a little effect on the hydrogen bonding structure and dynamics of aqueous NMA solution. The calculated self-diffusion coefficient values for water and osmolytes are in very good agreement with experimental observations [4-7].



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