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Theoretical study of hydration free energy of the C_{60}, $Li^+@C_{60}$, $Na^+@C_{60}$ and $K^+@C_{60}$

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Abstract: Fullerene (C_{60}) and endofullerene (a chemical specie trapped into C_{60}) are a molecule class largely explored to be used in chemical, medicine, biology, and others. Although the fullerene has been known since 1985, its solvation process in water is not clear in the literature. For example, there is not a consensus if the hydration free energy ($\Delta G_{hyd.}$) of the C_{60} is less or greater than zero. Therefore, in the present work, molecular dynamics (MD) technique was used to study the solvation process of the C_{60} and it complexed with the Li^+, Na^+ and K^+ ions, with goal to improve its solubility. All simulations were performed in the GROMACS 5.0.7 package [1]. The Lennard-Jones parameter developed by Girifalco [2] was used for C_{60}, the electrostatic parameters (charge) of the endofullerenes (ions@C_{60}) were obtained in previous work [3] using DFT//B3LYP/6-31G(2d,2p), and water solvent was described by the SPC model. The hydration free energies were calculated using the thermodynamic integration (TI) method. The structural analysis along 5 ns of MD simulations show that the ions trapped on C_{60} does not alters the overall solvation process, and the local structure of water molecules around the solute is preserved. The following $\Delta G_{hyd.}$ values were obtained: C_{60} (–32.5) > $Li^+@C_{60}$ (–132.0) > $K^+@C_{60}$ (–136.0) > $Na^+@C_{60}$ (–143.0 $kJ.mol^{-1}$). Our $\Delta G_{hyd.}$ value of the C_{60} agree reasonably with theoretical calculations (–36.6 $kJ.mol^{-1}$) [4] and with experimental data (–24.45 $kJ.mol^{-1}$) estimated by Luzhkov [5]. For all endofullerenes, our $\Delta G_{hyd.}$ values are in agreement with B3LYP/LANL2DZ/PCM calculations [6]. Overall, the present results can contribute to understand the solvation process of C_{60} and endofullerenes ions@C_{60}.

Key-words: hydration free energy, endofullerene, molecular dynamics simulation
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