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Original Research Article

Theoretical Studies of Interaction Melphalan Anticancer Drug with Functionalized Carbon Nanotube: Thermodynamics Studies

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ABSTRACT

One of the advancements of the present century is the use of carbon nanotubes in the treatment of cancer. As the carbon nanotubes pass through the cell wall, the anticancer drug is transferred to the cancer tissue and released. The purpose of this project is to obtain the thermodynamic functions and potential energy of the interaction between melphalan anticancer drug and functionalized carbon nanotube. The potential energy of this interaction is obtained by Monte Carlo simulation at different temperatures in the gas, methanol and water phases and the thermodynamic functions of this interaction is obtained by quantum mechanics by the density function theory with B3LYP/6-311G basis set at different temperatures in the gas, methanol and water phases. The results show that the Gibbs free energy and entropy are a function of the solvent dielectric constant. So that the Gibbs free energy and entropy changes of reaction are decreases and increases respectively. Also the results of both methods indicate that the best environment for this interaction is water solvent.

Keywords: Monte Carlo simulation, melphalan, interaction, carbon nanotube, Thermodynamic

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