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Original Research Article

Adsorption of Procarbazine Anti-cancer Drug on the Surface of Graphene: A DFT Study

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ABSTRACT

The present study aimed to assess the adsorption of graphene with anticancer drug procarbazine in a gas and solvent phase (water) at the B3LYP/6-31G (d) theoretical level. Initially, the structures of procarbazine and graphene complexes were optimized in three configurations. Afterwards, IR calculations and molecular orbital analysis were performed. In addition, some important parameters were assessed, including the adsorption energy, Gibbs free energy changes (ΔGad), enthalpy (ΔHad) variations, thermodynamic equilibrium constant, specific heat capacity, chemical hardness, energy gap, and electrophilicity. According to the results, Gibbs free energy changes (ΔGad), enthalpy (ΔHad) variations, I-Isomer and II-Isomer and III-Isomer were negatives at various temperatures, throughout the temperature range of 298.15-310.15 K. Since according to the obtained results for adsorption of procarbazine on the graphene in I-Isomer and II-Isomer and III-Isomer were spontaneous at various temperatures, throughout the temperature range of 298.15-310.15 K. Structural properties calculated, including the density and length of C-N bonds, and the findings of the analysis of molecular orbitals indicated that the reactivity, electrophilicity, and conductivity of procarbazine are reduced after this reaction. Also the calculated specific heat capacity values indicated that graphene could be utilized as a sensing material in the construction of thermal biosensors for procarbazine determination.

Keywords: Procarbazine, Anticancer drugs, Functional density theory, Graphene

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