عنوان مقاله:

Investigating the performance of nano structure C60 as nano-carriers of anticancer cytarabine, a DFT study

محل انتشار:

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خلاصه مقاله:

In this research study, stability, chemical properties, and thermodynamic parameters nano-derivatives of the cytarabine with the fullerene C60 nanostructure were calculated in the range of 298.15-310.15 K at the B3LYP/6-31G* level of theory. Possible isomers of the cytarabine (four different configurations) with C60 molecule were considered, and the effect of temperature on the thermodynamic parameters was studied. The adsorption energy, Gibbs free energy changes (ΔGad), enthalpy (ΔHad) variations, thermodynamic equilibrium constant, specific heat capacity, chemical hardness, energy gap, and electrophilicity were evaluated, as well. The results indicated that the adsorption of the cytarabine with fullerene C60 is spontaneous. In addition, the calculated specific heat capacity values revealed that, the C60 can be utilized as a sensing material in the construction of thermal biosensors for cytarabine determination.

کلمات کلیدی:

Cytarabine, fullerene C60, Nano drug, Density functional theory