Study of Adsorption Properties of Pipobroman the Surface of Carbon and Boron Nitride Nanotubes Using Density Functional Theory

Farzad Gholinea Loohesara*,

In recent years, using of nanotube as nano drug carriers has been investigated. In this investigation, two nanotubes as drug carriers of pipobroman line has been used, first of all the drug molecule structure pipobroman and nanotube modeler and and gauss view softwares then calculated by Gasussian 09 with DFT B3LYP 6-31G(d) method after these levels molecule pipobroman two sides of hetro atomic,oxygen and Br puted on different nano leves and calculated with below methods. The results was include energy connection informations such as dipolar, basic attributes(potential ionization,electron collective,chemical potential, hardness, softness) and in energy gaps in HOMO-LUMO, has been analysis and below results collected. point of view conection energy and attract amount(C) CNT(5,5) and pipobroman(Br) is best inter active with drug molecules pipobroman Br atom and dipolar point of view nanotube (e) BNNTdoped Ga and pipobroman(Br) have most dipolar pipobroman molecules, structure of this nanotube with pipobroman molecules (specially Br atom) have show pole acceptable and transportation more charges rather other structures.

Keywords : nanotubes, pipobroman, Gasussian 09, anti cancer drug