Research Article

Chemical Review and Letters
journal homepage: www.chemrevlett.com
ISSN (online): 2645-4947 (print) 2676-7279

Procarbazine adsorption on the surface of single walled carbon nanotube: DFT studies

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ARTICLE INFO

Article history:
Received 31 May 2020
Received in revised form 10 July 2020
Accepted 14 July 2020
Available online 22 July 2020

Keywords:
Procarbazine
DFT
Carbon nanotube
Adsorption

ABSTRACT

In this research, the performance of single-walled carbon nanotube (SWCN) as a sensor and nanocarrier for procarbazine (PC) was investigated by infra-red (IR), natural bond orbital (NBO), frontier molecular orbital (FMO) computations. All of the computations were done using the density functional theory method in the B3LYP/6-31G (d) level of theory The calculated negative values of adsorption energy, enthalpy changes, Gibbs free energy changes showed the PC interaction with SWCN is exothermic, spontaneous and experimentally possible. The increasing of specific heat capacity (C_V) of SWCN after adsorption of PC showed the thermal conductivity improved during the interaction process and this nanostructure is an excellent sensing material for the detection of PC. The NBO results demonstrate in all of the evaluated conformers a chemical bond with SP^3 hybridization is formed between the medicine and SWCN. The great values of thermodynamic constants showed the adsorption process is irreversible and SWCN is not a suitable nanocarrier for delivery of PC. The density of states (DOS) spectrums showed the bandgap of SWCN decreased sharply after the adsorption of PC and this nanomaterial can be used as a sensor for electrochemical detection of PC.

1. Introduction

Procarbazine (PC) which its optimized structure is given in the Figure 1, is a cytotoxic chemotherapeutic medicine that is prescribed orally for the treatment of lymphomas and brain tumors. PC was approved for the first time in 1969 and it is on the WHO list of essential medicines [1-5]. PC has high toxicity and severe adverse effects like bloody vomit, fever, unusual bleeding or bruising, hallucinations, fainting, nervousness, depression, lethargy and liver malfunction. In this regard, finding a new nanocarrier and detection method for PC is very important [6-8]. On the other hand, single-walled carbon nanotube (SWCN) is an allotrope of carbon. This nanostructure consists of a cylindrical graphene sheet with a length of about a few microns and a diameter of 0.4 to 2 nanometers (Figure 1). SWCN has unique features, including high surface-to-volume ratio, high thermal conductivity, medium electrical conductivity and high tensile strength [9-13]. And these outstanding properties have led to the application of this nanomaterial in various fields such as biosensors and sensors, removal of environmental contaminants, drug delivery, super-capacitors and the development of new extraction methods [14-17]. In this regard, it was decided to investigate the performance of SWCN as a novel nanocarrier and sensor for drug delivery and determination of PC for the first time by IR, NBO and FMO computations.

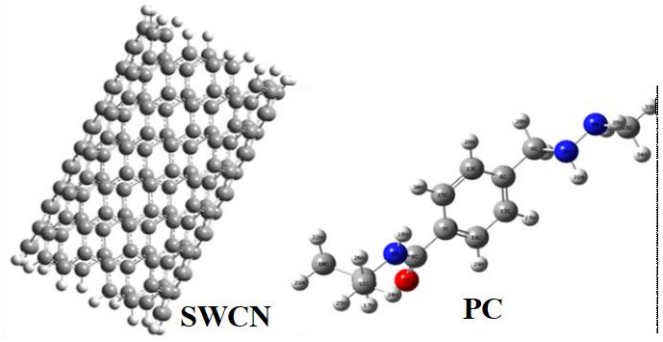

Figure 1. Optimized structures of PC and SWCN