4TH National Conference of Iran Chmistry, Chemical Enginereeng And Nano

Adsorption of 2- methyl-N-(2′-aminoethyl)-3-hydroxyl-4-pyridinone onto functionalized single-walled carbon nanotube: A DFT study

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Abstract

In this work, the interaction of 2- methyl-N-(2′-aminoethyl)-3-hydroxyl-4-pyridinone (MAEHP) drug with (7,0) armchair single-walled carbon nanotube (SWCNT) was investigated on the basis of density functional theory (DFT) at the B3LYP/6-31G(d) level of theory. DFT calculations revealed that the binding energy of SWCNT-MAEHP complex is negative, suggesting thermodynamic favorability for covalent attachment of functional moiety onto nanotube sidewall. The quantum chemical reactivity indices indicated that the reactivity of SWCNT-MAEHP complex increased in comparison to pristine nanotube and MAEHP drug. These results are extremely relevant in order to identify the potential applications of functionalized carbon nanotubes as drug delivery systems.

Keywords: Carbon nanotubes, MAEHP, DFT, Reactivity descriptors, Drug delivery.

1. INTRODUCTION

MAEHP is an effective metal chelator, which has high affinities for iron, aluminium, cooper and zinc [1]. This selective chelation property makes it a suitable choice for the treatment of Alzheimer and iron overload disease [2]. It is one of the deferiprone (DFP) derivatives, which can decrease excess iron, aluminium, cooper and zinc without effecting the essential elements such as calcium and manganese [3]. Carbon nanotubes (CNTs) belong to the family of fullerenes, which are third allotropes of carbon after graphite and diamond [4]. Because of their physicochemical properties, they are important in the field of biomedical and drug delivery systems[5]. MAEHP is conjugated to CNTs through the formation of an amino bond between a primary amino group in the drug and a carboxyl group on the CNT surface [6]. Theoretical studies help us to understand, chemical reactivity, stability of CNT-drug complexes and drug uptake mechanism by CNTs [7]. The present work indicates the density functional theory (DFT) calculations on the binding energy and stability of CNTs upon covalent functionalization with –COH functional group and subsequent loading with MAEPH molecule.

2. COMPUTATIONAL METHODS