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Exploring Benefits of a Be-Doped Carbon Nanocone for the Drug Delivery of 2-Thiouracil: Computational Study

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Abstract: By the importance of employing nanostructures in therapeutics, a model of beryllium (Be)-doped carbon nanocone (BNC) was explored in this work for the drug delivery of 2-thiouracil (2TU). Density functional theory (DFT) calculations were performed to recognize the stabilized structures in single and complex states. Six models of BNC-2TU complexes were obtained with different levels of interaction strengths, which were all reasonable levels of strength for the formation. In each model, a characteristic relaxation configuration of BNC and 2TU substances was observed with a deterministic role of defining strength levels and electronic features. Be…S, Be…O, and C…H were the types of observed interactions in the complexes with complementary roles of enhancing the strength of complexes. Localizations of molecular orbitals patterns were also dependent on the relaxation configurations of complexes; localization at both interacting sides or only one side was observed for the models. Indeed, obtaining such various features made the complexes flexible models for employing the desired functions and purposes. Formations of all models were suitable regarding the values of interaction energies; the obtained configurations and features could make them appropriate complexes for approaching desired functions such as drug delivery processes.

Keywords: nanocone; 2-thiouracil; adsorption; drug delivery; density functional theory.

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1. Introduction

After the pioneering innovation of carbon nanotubes in 1991, several efforts have been dedicated to learning features of novel nanostructures to develop their desired applications [1-5]. A characteristic feature of high surface area made nanostructures suitable surfaces for working as an adsorbent in adsorption processes [6-10]. The pure carbon-based nanostructures were almost the first innovative nanostructures, but their modifications and heteroatomic compositions were achievable for these novel materials [11-15]. Existences of low-concentration atomic impurities could make atomic doped nanostructures with the suitability of heteroatomic regions for conducting the adsorption processes [16-20]. In this regard, several efforts have been dedicated to this time to make different atomic doped or molecular functionalized nanostructures regarding their suitability for desired purposes and processes [21-25]. Additionally, other geometrical shapes of nanostructures besides the original tubular

shape were found in the category of nanostructures, such as fullerene, graphene, and nanocone [26-30]. It should be noted that the shape of the nanostructure could make it a characteristic material for participating in the desired processes [31-35]. The synthetic processes have found the original nanocone as a conical shape with the carbon atoms compositions [36]. After that synthetic innovation, the nanocones have been topics of considerable research work up to now for developing their new applications [37-40]. The apex tip of nanocones is an important site for conducting communications with other external substances with specific features for developing applications, especially in interactions with other substances [41-45]. During the last three decades, several biomedical applications were developed for the nanostructures in single-standing nano-systems or combinations with other chemical and biochemical systems [46-50]. One of the major expected applications of nanostructures is their significant role in targeted drug delivery platforms [51-55]. In this regard, several efforts have been made to enhance the medical platforms with the assistance of nanostructures from the time of nanotechnology innovation up to now [56-60]. Accordingly, the benefits of a model of beryllium (Be) doped carbon nanocone (Figure 1) were explored in this work for employing in the drug delivery of 2-thiouracil (Figure 2).

2-Thiouracil (2TU) has been known as an anti-thyroid drug for several years by inhibiting the activity of the thyroid peroxidase enzyme [61-65]. Because of its important therapeutic features, several works were done to enhance this drug's efficiency for approaching better treatment levels [66-70]. Indeed, exploring novel treatments for known and unknown diseases is very important to maintain the balance of the human health system [71-75]. Accordingly, developments of both new drug substances and new drug treatments are essential for approaching therapeutic purposes [76-80]. As explored in the current work, combining a drug with nanostructures is one way of approaching an enhanced drug delivery platform [81-85]. To this aim, combinations of a Be-doped carbon nanocone and 2-thiouracil drug (Figure 3) were explored in this work to learn the benefits of formations of such complex systems for approaching a targeted drug delivery platform. To achieve the goals of this work, computational chemistry tools were employed to obtain structures and their related features [86-90].

2. Materials and Methods

This work was done using density functional theory (DFT) calculations at the B3LYP-D3/6-31G* computational level as implemented in the Gaussian program [91]. The calculations were done in two steps optimizing the geometries first and evaluating the features next. The models of single Be-doped carbon nanocone (BNC) (Figure 1) and 2-thiouracil (2TU) (Figure 2) were optimized to be prepared for participating in the interaction processes. Based on the examinations of all possible interaction situations of BNC and 2TU, six models of BNC-2TU complexes were obtained as designated by C1 to C6 (Figure 3). All the complex configurations were obtained by optimization calculations, and additional describing features were evaluated. As listed in Table 1, the strengths of interactions were analyzed using the evaluated features of the quantum theory of atoms in molecules (QTAIM) [92-94]. In this step, all involving interactions between the substances of complexes, as shown in Figure 3, were identified based on each energetic and distance magnitudes. Moreover, the differences in total energies of complexes and each of the interacting substances were obtained by the strengths of molecular interaction energies. Types of interactions and their distances (DIS), total electron density (RHO), Laplacian of electron density (DEL^2-RHO), energy density (H), and interaction

energy (E_I) were all summarized in Table 1. It is worth to note the calculated values of basis set superposition error (BSSE) were almost negligible to be considered in the evaluations of values of E_I. Next, the contents of Table 2 were provided by the values of molecular orbitals energies emphasizing the values of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) and their related features, such as energy gap (E_G) and chemical hardness (CH). Besides the evaluated quantities, graphical representations of HOMO and LUMO were exhibited in each of Figures 1-3 for the optimized geometries of the obtained models to show localization concentrations of molecular orbitals on the molecular sites. As a consequence, the models were available by the optimized geometries and the evaluated describing features for exploring the benefits of BNC for the drug delivery of 2TU.

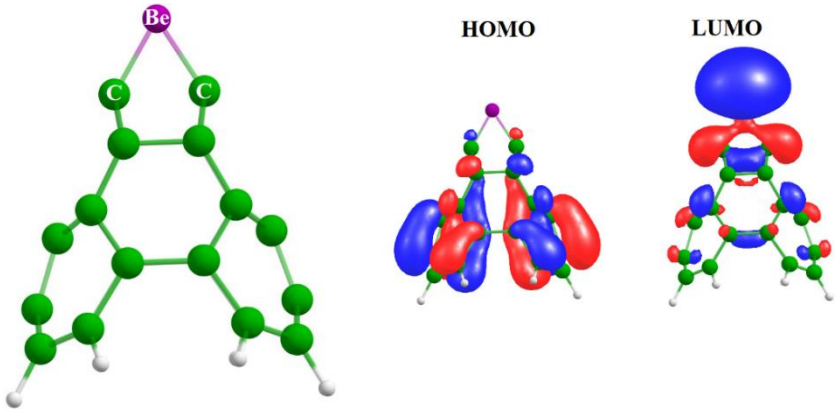

Figure 1. The optimized model and HOMO-LUMO representations of single BNC.

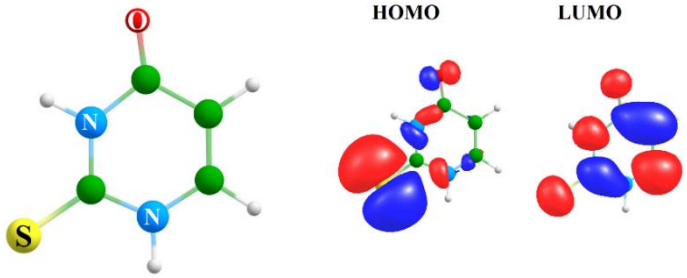

Figure 2. The optimized model and HOMO-LUMO representations of single 2TU.

3. Results and Discussion

Exploring the benefits of employing a beryllium (Be) doped carbon nanocone (BNC) for the drug delivery of 2-thiouracil (2TU) was investigated in this work by means of performing DFT calculations. As shown in Figures 1 and 2, the single models were optimized to be prepared for participating in interactions with each other. For the BNC model, one Be atom was substituted at the tip of the nanocone to provide an interacting site for the structure. On the other hand, all possibilities of interactions of 2TU through its atomic sites were examined for participating in interactions with the adsorbent. Accordingly, six models of BNC-2TU complexes were obtained by performing optimization calculations as shown in Figure 3; C1-C6 complexes. It is worth mentioning that the obtained BNC-2TU complexes were obtained by examining all possibilities of interactions between BNC and 2TU substances, in which six complexes were obtained. To make a deep analysis of the complexes, details of interactions were investigated by performing additional QTAIM analysis on the optimized BNC-2TU complexes.

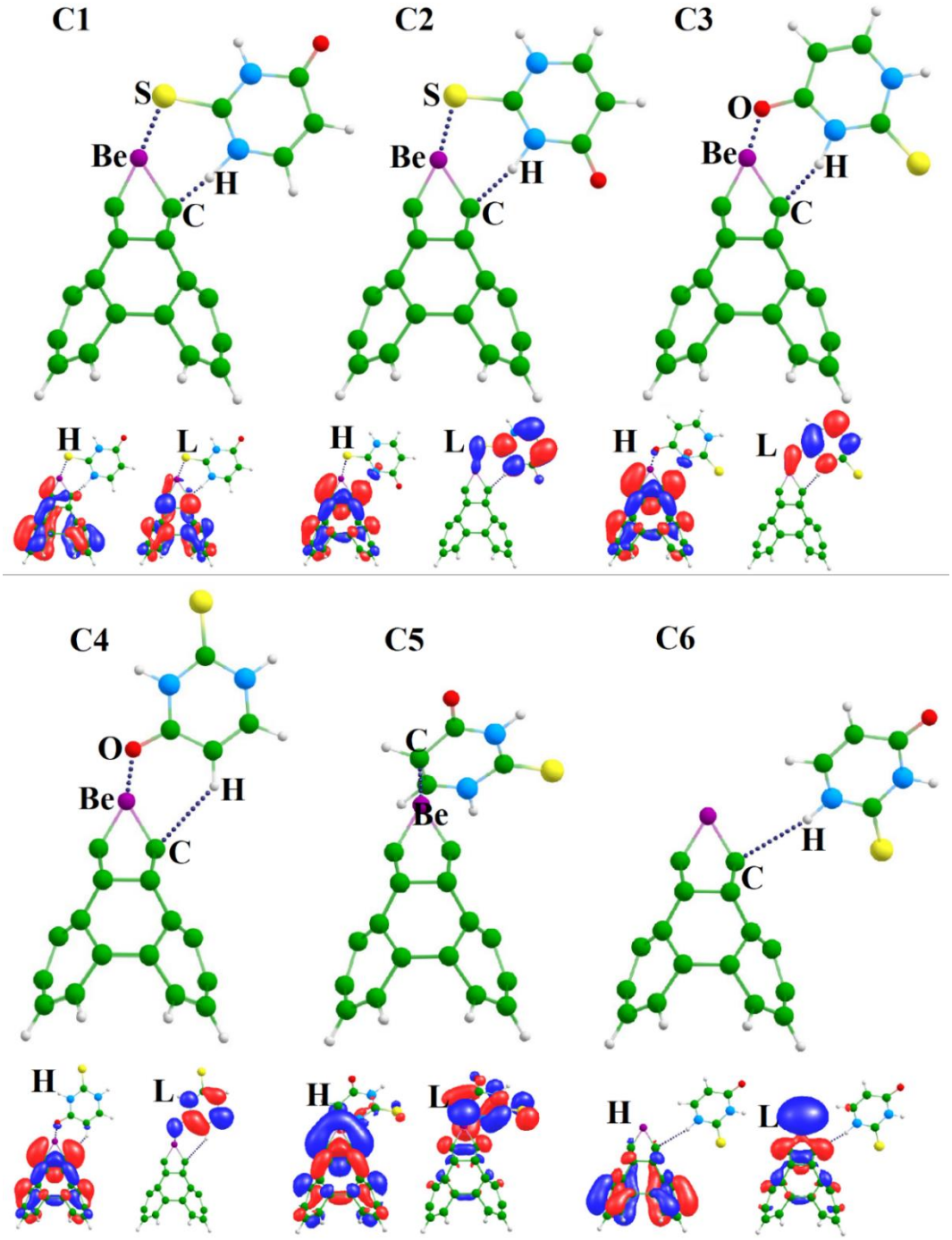

Figure 3. The optimized models and HOMO-LUMO (H and L) representations of complexes of BNC-2TU.

Table 1. Interactions features.[1]

BNC-2TU	INT	DIS (Å)	RHO (au)	DEL^2-RHO (au)	H (au)	E_I (kcal/mol)
C1	Be…S C…H	2.014 1.451	0.074 0.068	0.188 0.037	-0.051 -0.022	-50.129
C2	Be…S C…H	2.006 1.748	0.069 0.058	0.204 0.069	-0.019 -0.011	-42.344
C3	Be…O C…H	1.546 1.745	0.094 0.061	0.719 0.069	-0.064 -0.012	-50.968
C4	Be…O C…H	1.579 2.599	0.082 0.013	0.633 0.033	-0.019 -0.011	-45.581
C5	Be…C	1.885	0.056	0.179	-0.014	-17.626
C6	H…C	2.595	0.009	0.025	-0.001	-2.672

[1]The models were shown in Figure 3.

The involved interactions of Figure 3 were known by the obtained QTAIM results, in which their detailed quantitates were summarized in Table 1. A quick achievement of the obtained results is that the Be-doped region worked as an interaction environment manager to manage interactions between BNC and 2TU substances. In all complex cases, the models communicated with each other through the Be-doped atom directly or its neighboring carbon atom indirectly. Additionally, the idea of Be-doping of nanocone was affirmed by a significant contribution of Be atom of BNC substance to interactions with the 2TU substance. In this regard, the models were stabilized, and their features were investigated in terms of geometries and energies to show the benefits of formations of such BNC-2TU complexes. To this point, the models of complexes were also comparable to each other regarding their priority of formation. As described in Table 1, the complex models of Figure 3 were in different levels of strength of interactions, and different configurations were obtained. The important point is that the interactions were all in the physical mode of non-covalent type, and their strengths were reasonable. Another important point is that the existence of C…H interaction was observed in the complexes. Additionally, different configurations and their corresponding strengths showed the importance of examining all interacting configurations to approach complex formations. Based on the obtained values of EI, the strength order of interacting complexes was found to be C3 > C1 > C4 > C2 > C5 > C6. In this regard, the obtained strengths showed the importance of the relaxation configuration of two counterparts towards each other and the characteristic role of their involving interactions. Accordingly, both of Be…S and Be…O interactions were stronger by the existence of additional C…H interactions. As a consequence, formations of BNC-2TU complexes were found suitable for approaching the role of adsorbent for the BNC substance towards the 2TU substance.

Table 2. Molecular orbitals features.[1]

Model	HOMO (eV)	LUMO (eV)	E_G (eV)	C_H (eV)
BNC	-5.241	-2.709	2.532	1.266
2TU	-6.315	-1.604	4.711	2.356
C1	-5.060	-2.246	2.814	1.407
C2	-4.536	-2.413	2.123	1.061
C3	-4.491	-2.920	1.571	0.785
C4	-4.067	-3.424	0.644	0.322
C5	-4.757	-3.254	1.502	0.751
C6	-5.476	-3.159	2.316	1.158

[1]The models are shown in Figures 1-3.

Molecular orbitals of the optimized modes were exhibited in Figures 1-3, and their quantities were summarized in Table 2 based on the consideration of HOMO and LUMO levels. Indeed, the frontier molecular orbitals play important roles in determining the electronic features of molecular models, especially within their participation in electronic transferring processes. To this aim, such features were evaluated for the models of this work to describe their electronic-related properties. As shown in Figure 1, a significant concentration of LUMO at the Be-doped region of BNC made it a suitable region for participating in interactions through the lone pairs of electrons of S and O atoms of 2TU. Accordingly, the models of C1 to C6 showed different configurations of HOMO and LUMO patterns based on different configurations of relaxations of two interacting BNC and 2TU substances. In the cases of C2, C3, C4, and C5, patterns of HOMO and LUMO were separated with the HOMO localization at the BNC part and the LUMO localization at the 2TU part. In the case of C1, both of HOMO and LUMO were localized at the BNC part. And in the case of C6, a model of pattern localization similar to the original single BNC was observed. In this regard, the models were

distinguished based on their electronic features with deterministic roles for their future applications in the drug delivery processes. In addition to these graphical representations, the evaluated quantities of Table 2 showed different features between single and complex models. The levels of HOMO and LUMO were significantly changed from single to complex states, besides observing significant variations among the complex models. Accordingly, the values of E_G and C_H were changed regarding the changes in HOMO and LUMO levels. It is obvious that the formation of BNC-2TU complexes had impacts on the electronic features, in which the model of configuration relaxation of BNC and 2TU towards each other was dominant for observing the molecular orbital-based features. In this regard, the desired function could determine the advantage of each complex formation for approaching the goal.

4. Conclusions

To summarize this work's achievements, an important point is the reasonable formation of BNC-2TU complexes regarding the obtained levels of interaction strengths. Additionally, six possible configurations were obtained for the complexes regarding the relaxation of each of the BNC and 2TU substances towards each other. The Be-doped region was a dominant site of interactions for the BNC substance to manage formations of complexes. Regarding the graphical and quantitative features of molecular orbitals, the impacts of such relaxation configurations of complexes were observed for the models. Localizations of each of the HOMO and LUMO patterns at each molecular side or both molecular sides were determined by changes in relaxation configurations. Accordingly, the models were found flexible for approaching the desired function, such as conducting the drug delivery processes.

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Conflicts of Interest

The authors declare no conflict of interest.

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