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THEORETICAL STUDY OF THE B20P20 FULLERENE-LIKE NANOCAGE DRUG CARRIER VIA DFT

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Abstract

This study examined the theophylline drug's adsorption onto the outer surface of fullerene-like nanocages, such as B20P20. Our calculations indicate that theophylline attaches to the B20P20 nanocages utilising calculations grounded in the quantum theory of atoms in molecules (QTAIM) and density functional theory (DFT),. Subsequently, B20P20 nanocages containing C7H8N4O2 theophylline bind the medication. Their bandgap (Eg) values dropped as a result of the theophylline drug adsorption onto the aforementioned nanocages, which increased their electrical conductivity by changing the energy levels of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO).. All of the mentioned nanocages have shown promise as electronic sensors and as possible vehicles for theophylline medication delivery in living organisms, according to this trend. Total energies, electronic states, energy gaps, ionisation potentials, chemical potential, electron affinities, global hardness, softness, and global electrophlicity were computed, along with the optimised structure. Frequencies of harmonic vibrations computed and compared with existing experimental evidence. The findings demonstrated an enhancement in electrical characteristics and a reduction in gap energies.

Keywords: *DFT, Fullerene-like nanocages, nanostructures.*

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Introduction

The biosphere was the ideal setting for the use of nanoparticles because of its unique properties, which include size, hydrophobicity, aggregation, chemical composition, shape, and surface charge density. (1). Research into nanoparticles and nanostructured materials is only one example of the many scientific fields that have made great strides recently (2). Nanotubes, nanocages, and nanoclusters are just a few of the nanostructures that have just emerged as promising components for chemical sensors and drug delivery systems of the future (3).

The electrical conductivity and other electronic properties of the resultant complex are influenced by the electron exchange between the adsorbed molecules and the nanomaterials. This might be seen as a signal for a potential sensor. in (4). Nanocages are an attractive class of nanostructures due to their unusual physical and chemical properties, such as a small HOMO-LUMO band gap (5) and fullerene-like materials. Ones have the most stable structures, according to the literature review, out of all the fullerene-like structures (6). If you suffer from wheezing, shortness of breath, or chest tightness as a result of asthma, chronic bronchitis, emphysema, or another lung illness, theophylline may help. Relieving stress and opening up the airways of the lungs, it facilitates easier breathing. (7). Proteins and other target tissues are among the many entities with which this molecule can interact. (8). Theophylline and its derivatives have been the subject of several investigations; nevertheless, in order to investigate theophylline's interaction with BP fullerene, the energetic, geometrical, and electrical properties were determined using B3LYP techniques.(9) Theophylline may have interacted with the surface and wall of the tube after being physically or chemically absorbed. (10) They proved that the interaction mechanism proves the electronic properties of the nanostructures. (11) gradually transformed Through the application of density functional theory, this research aims to explore the possibility of chemically functionalizing B20P20 with a theophylline molecule.Nanocages are materials that resemble fullerenes; in this article, we intended to investigate their potential use for the administration of theophylline (13). Here, all drug-nanocage geometries have their structures, energies, electrical structures, and stabilities measured using DFT and QTAIM simulations.. (14) Future experimental research aimed at creating medication delivery techniques will build on the results of this work, Prior research: this study adds to the existing body of knowledge by providing new data on 5furacil - InGaP Diamantane Nanocrystals for optimisation of shape and total energy calculations.(15)

2. Computational details

2.1. DFT calculations

The software package Gaussian 09 was used for all mathematical operations. (16). Researchers looked at how theophylline interacted with B20P20 nanocages by using quantum chemical computations.(17) Theophylline molecule and all complex and pure nanocage designs were analyzed using density-functional theory (DFT) with the B3LYP/6-311G method/basis set. (18) . It seems feasible to model $X_{20}Y_{20}$ systems at this theoretical level.

that year (19).Along with that, a number of quantum molecular parameters (20) like the ionization potential (I.P= -E_{HOMO}), the molecule's electron affinity (E.A = -E_{LUMO}), the system's chemical potential (μ = - (I.P+E.A)/2), hardness (η = (I.P- E.A)/2), softness (S=1/2η), and the electrophilicity index ($\omega = \frac{\mu^2}{2\eta}$) are also important.

2.2. Atoms in molecules (AIM) calculations

The state-of-the-art electrical structures modelling capabilities of the Gaussian 09 software can be enjoyed on a variety of computer systems. (21).In addition to state-of-the-art tools for electrical structure modelling, the Gaussian 09 licence covers a wide range of computer platforms. The number 22.

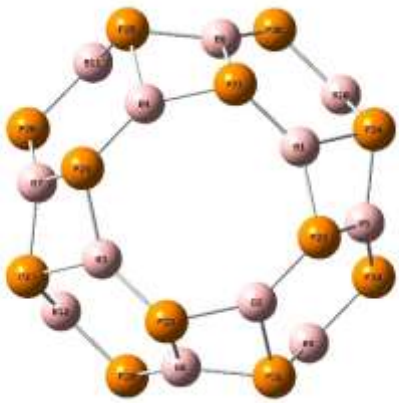
While developing Gaussian, we kept the user's needs in mind. The input is completely free-format and mnemonic, the defaults are acceptable, and the output is supposed to be rather self-explanatory.. [23]. Advanced users have the option to adjust default settings or integrate their own code with the Gaussian system [24]. Instead than worrying about the nuts and bolts of doing the calculations, the authors hope their work will free users to concentrate on coming up with novel solutions and using the methodology to real-world chemical challenges. [25].

3. Results and discussion

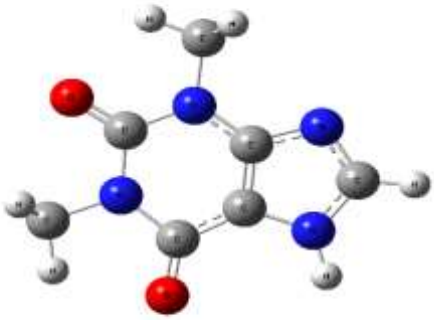
Table 1. listed the C7H8N4O2 theophylline molecule, B20P20 nanocages, complexes C7H8N4O2-adsorbed B20P20 nanocages, chemical potential (l), electrophilicity index (x), ionisation potential (I), Fermi level (EF), and electron affinity (A) .

property	theophylline	$B_{20}P_{20}$ nanocages	Complexes A1
E_{HOMO}(eV)	-5.19	-6.39	-4.95
E_{LUMO}(eV)	-1.72	-3.10	-3.09
Eg (eV)	3.47	3.29	1.85
E_F	-3.455	-4.745	-4.02
I.P	5.19	6.39	4.95
E.A	1.72	3.10	3.09
η	1.73	1.64	1.85
μ	-3.45	-4.74	-4.02
S	0.29	0.30	0.54
ω	3.44	6.83	4.48

a-



b-



c-

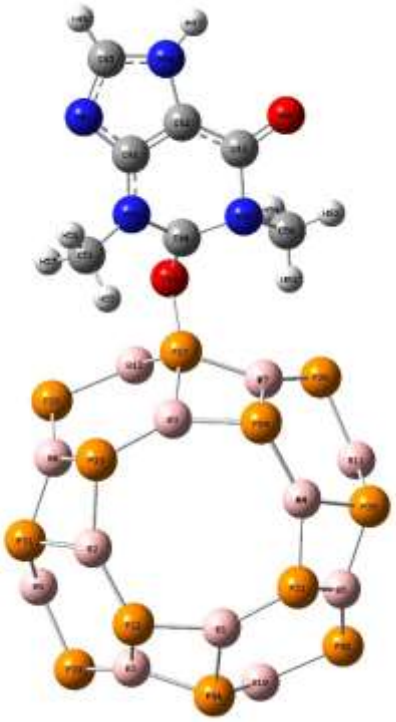
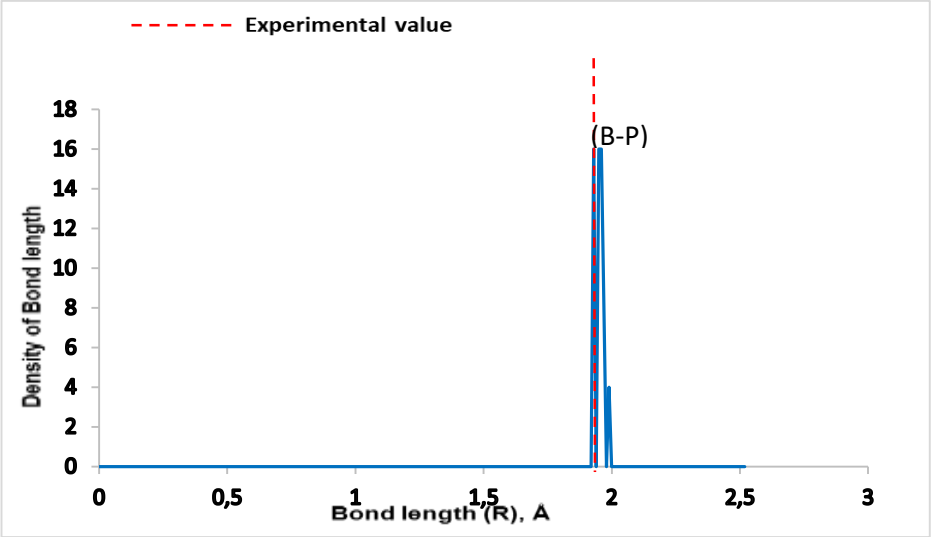
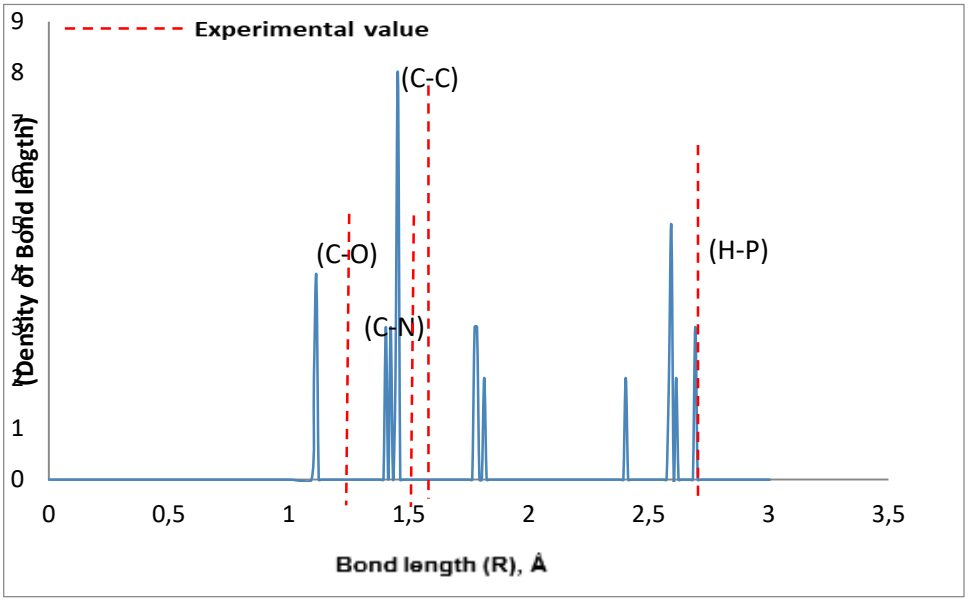


Figure 1.Shows a theophylline molecule with an optimised structure: C7H8N4O2. Theophylline-adsorbed B20P20 nanocages b-complexes with C7H8N4O2. The coordinates are in A.

The structure's optimisation Eight 6-membered rings (6-MR) and six 4-membered rings (4-MR) make up a B20P20 cage in the ideal B20P20 cluster configuration. Two of the B-P bonds are 6-MRs, while the other is shared by a 4- and a 6-MR. A molecule's bond length is the average distance between two bonded atoms' nuclei. Figure 1 also shows that we investigated the possibility of creating an endohedraly B20P20 nanocage complex.The molecular geometry is defined by the relative configuration of the atom's orbitals as they pass through its core. [26] shows the nanocage in its fully relaxed ground state. For every perfect nanocage, the equilibrium bond length B-P is shown in Fig.1





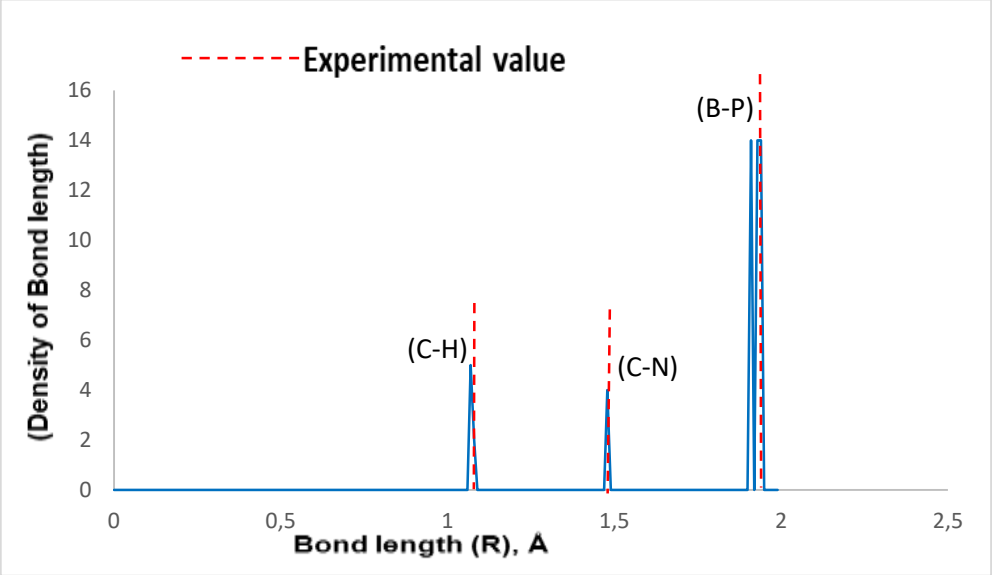
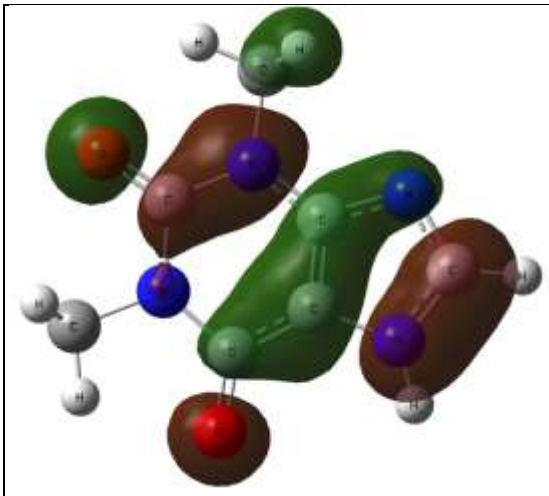


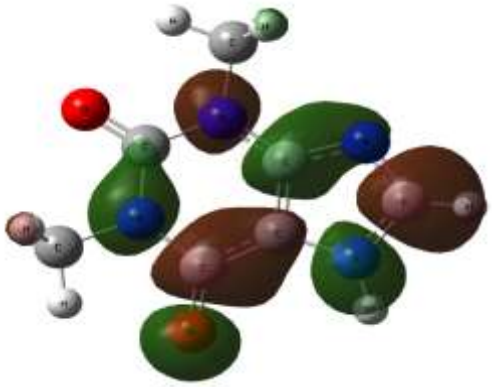
Figure 2. A theophylline molecule with an optimised structure: C7H8N4O2. Theophylline-adsorbed B20P20 nanocages b-complexes with C7H8N4O2. The coordinates are in A.

The molecular orbitals, which are a product of the linear combination of atomic orbitals, are the source of the HOMO and LUMO surfaces. New colours are seen in the HOMO and LUMO figures; green indicates the positive half of the wave function, and dark red indicates the negative half. According to this alternative explanation, the green colour represents the area of positive electrostatic potential, while the dark red colour represents the region of negative electrostatic potential. These two new colours have recently shown up in HOMO and LUMO figures. [27]

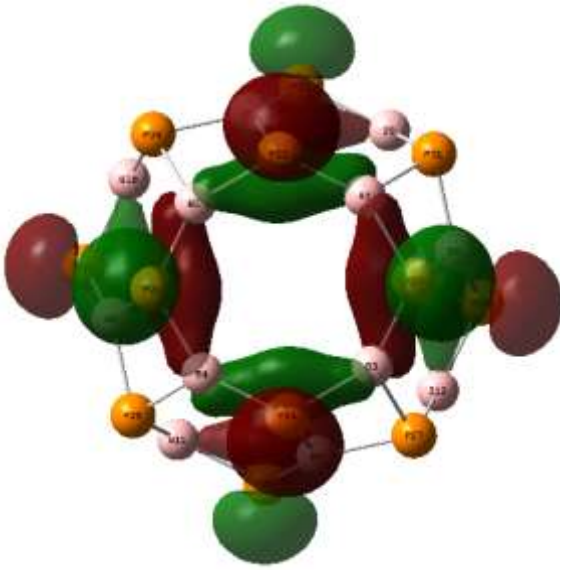
The distributions of HOMO and LUMO, as well as the fully relaxed ground-state structure of the nanocages, are shown in Figure 4.



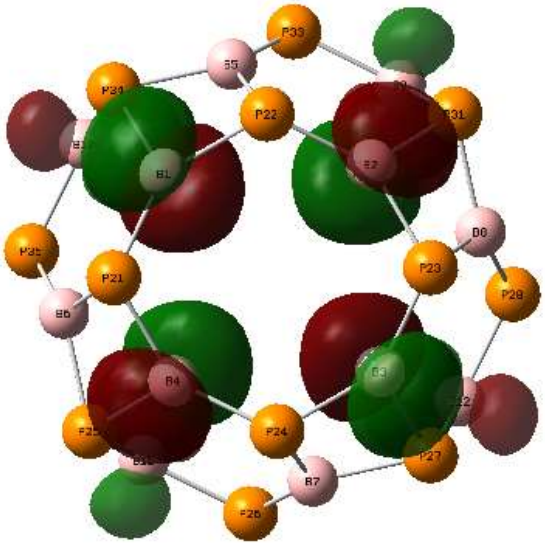
a-HOMO theophylline



a- LOMO theophylline



homo



Lumo

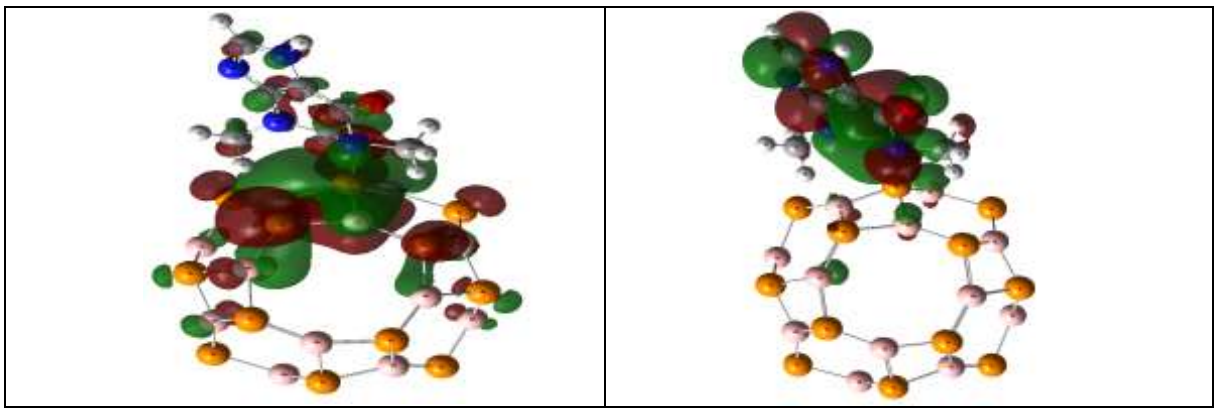


Figure 3 One molecule of theophylline, C7H8N4O2, b-B20P20 nanocages, and c-complexes of B20P20 nanocages adsorbed with C7H8N4O2, in their HOMO and LUMO orbitals. The coordinates are in A.

Conclusions

This work provides new data for the shape optimization, computed total energy, nanocage drug carrier. The studying of the electronic structure and vibration properties of carbon nanotubes as drug delivery using DFT .The ionization potentials are computed by the energy- vertical.Every medication that was arbitrarily chosen has a neutral substance that shows the surface's green color and stays there.

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