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A Computational Study on the Cisplatin Drug Interaction with $B_{24}N_{24}$ Fullerene

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Abstract
In this computational study, density functional theory with Gaussian 16 software was used to investigate the process of adsorption of the cis-Pt complex by Boron nitride ($B_{24}N_{24}$) nanostructures. Therefore, first, all structures were optimized by M06-2X method with two different base sets of Def2tzvp and also 6-31g (d) / LanL2DZ (base set LanL2DZ only for Pt atom). Then the amount of superposition error for the adsorbed cis-Pt complex on the Boron nitride nanostructure was measured and all electronic energies were modified. Our results show that the process of binding chlorine of cis-Pt complex to the Boron atom of the Boron nitride nanostructure is exothermic and also the adsorption type is physical because, at both computational levels, the adsorption energy of the process is less than 10 kcal.mol^{-1}.

Keywords: Cisplatin, Fullerene, Chemical Interaction

Introduction
Platinol is widely used to treat cancers including esophageal, bladder, ovarian, testicular, and brain tumors .Exposure to platinum or other soluble platinum compounds in hospital wastes poses a health risk because these substances are toxic and non-biodegradable.
Therefore, identifying and studying platinum drugs is an important issue. Conventional methods, which include gas chromatography and high-performance liquid chromatography methods, require precise tools.
Nowadays, the new class of sensors based on nanostructures are particularly popular due to their high surface-to-volume ratio. An important type of nanostructures based on BN units include nanotubes, nanoparticles, etc.
BN nanostructures have wide bandgap, stable oxidation resistance, high thermal conductivity and less toxicity .An important type of BN nanostructures that has attracted the attention of researchers is B24N24, which has been used for therapeutic purposes due to its biocompatibility. In this research, the main goal is to investigate the absorption and interaction of cisplatin drug on fullerene B24N24.
(Ohba et al, 2001) performed calculations on structural, dielectric and dynamic properties of BN network. They used fictitious potential and DFT techniques in their calculations .Lattice constant calculations and experimental values were in good agreement. The bulk model for the cubic and werzit structures is similar to diamond, but the h-BN structure is not hard and soft. The calculation results predict that the cubic structure is more stable than all the structures.
For the dielectric properties, the results obtained for the structures are in good agreement with the experimental values .The average value of dielectric constant and Bohr charge transfer in w-BN is similar to c-BN. However, Raman spectroscopic study easily distinguishes these two structures. On the other hand, the active peaks in Raman and IR of h-BN structures are different from c-BN and w-BN and h-BN structure can easily be distinguished from the other two structures.
(Liu et al, 2003) conducted a study on boron nitride structures using DFT-LDA method and found that the electronic properties of BN structures depend on the arrangement of their atoms.
The diversity of the band gap of the observed structures is due to the type of structural arrangements. In these investigations, it was found that irregular BN structures have a smaller band gap than h-BN structures.
(Li et al, 2006) conducted a study on the zigzag and armature structures of born nitride nanotubes using the GGA method. There is a significant difference in structure stability and energy gap between zigzag and armature forms. These differences are the basis for the difference in chemical and physical properties of these structures.
In this study, in addition to the differences between the armature and zigzag boron nitride structures, the thermal stability of aluminum nitride and its semiconducting properties were determined, which showed that the gap changes of these structures are related to their length changes.
The first fundamental calculations based on DFT showed a number of unusual properties of boron nitride functionalized with hydrogen and fluorine, whichh are different from functionalized graphite.
Unlike graphite, whichh becomes an Insulator by hydrogenation of metallic properties, with

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hydrogenation of BN, this bandgap structure is similar to the non-functionalized sheet.
In addition, the BN sheet can have a gap change from 4.6 to 0.6 and according to the amount of hydrogenated surface, it can have a direct, indirect and even semi-metallic gap.
Also, unlike the graphene sheet, the BN sheet, whichh has a heteroatomic structure, when treated with hydrogen or fluorine, can have anisotropy and magnetic properties with rich electrons. The magnetic stability of functionalized bornitride can be used for specific purposes and applications (Guth et al, 2009).

(Taherpour et al, 2018) during two separate researches, they designed two suitable gas sensors by using a cut BN monolayer and doping It with Sc and Y atoms to Increase the sensitivity to detect He inert gas. Using DFT and TD-DFT calculation methods, they obtained electronic changes including changes In the density of ground states and optical changes In UV-Vis absorption. Also, using NBO calculations, they evaluated the Interaction of this gas with the surface of the sensor (Taherpour et al, 2015).

Research method

In this research, density function theory and Gaussian 16 software were used to investigate the absorption process of cisplatin complex by boronitride nanostructure (B24N24).
Among the most important and perhaps the most widely used software in the field of computer use in chemical research is the powerful Gaussian software.
This software Is a set of interconnected programs that perform all kinds of quantum mechanics calculations. Gaussian's basis is based on the premise that theoretical models should be equally applicable to all molecular systems of any size and type.
Gaussian predicted the energy, molecular structures and vibrational frequencies of atomic or molecular systems by using the basic laws of classical or quantum mechanics.
It also provides molecular features obtained from various basic calculations.These features are useful for chemists, physicists, and other scientists who work In the growing and up-to-date fields of research In the areas of Interest in chemistry. This software provides the possibility of conducting virtual chemistry research with a reasonable cost and saving the time of testing In the laboratory.

Findings

The results of calculations and simulations in Gaussian software can be seen in figures 1 to 3. Also, the values of electronic energy (super position error) and dipole moment for the studied species are given in Table 1

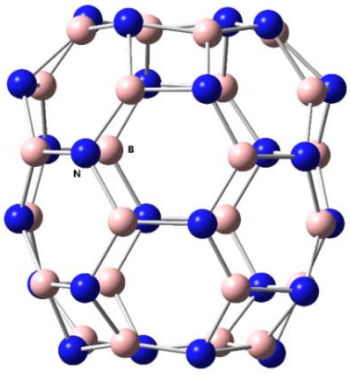

Figure 1: Optimized structure of B24N24 nanoparticle by MO62X/DF2TZVP method

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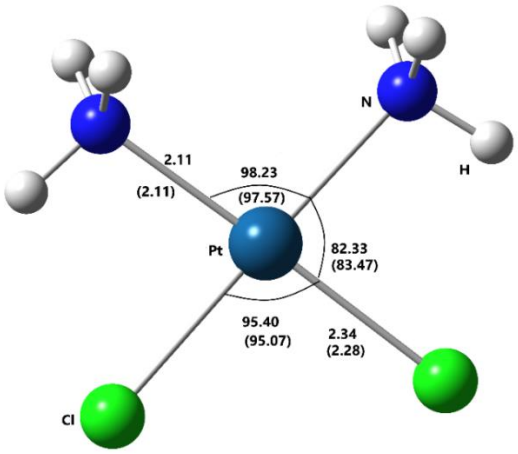
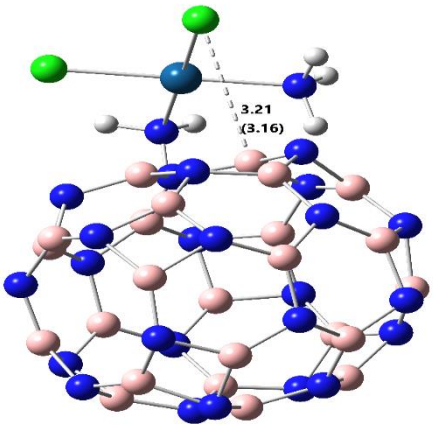


.Figure 2: Optimized structure of PTCL2(NH3)2 nano cisplatin using MO62X/DF2TZVP method

DF2TZVP base series (bond length in angstroms .and bond angle in degrees)

The numbers outside the parentheses are for the 6-31G(d)/Lanl2DZ base series and the numbers In the parentheses are for the



.Figure 3: Optimized structure of B24N24-Cis-PT complex by MO62X/DF2TZVP method

The bond length of Cl with Br is 3.21 angstroms for the 6-31G(d) basic series and 3.16 angstroms for the .DF2TZVP basic series

Table 1: Electronic energy values (super position error) and dipole moment for the studied species

	M062X/DF2TZVP	**M062X/gen/6-31G(d)//LanL2DZ**
E(B24N24)	-1912.2903425 (Hartree)	-1912.287293 (Hartree)
E(Cis-Pt(Cl)2(NH3)2)	-1152.864371 (Hartree)	-1152.775243 (Hartree)
E(B24N24)- Pt(Cl)2(NH3)2)	-3065.1415895 (Hartree)	-3065.051269 (Hartree)
ΔE(absorption)	-0.013124 (Hartree)	-0.011267 (Hartree)
BSSEs	0.001599063147 (Hartree)	0.0015789063147 (Hartree)
Dipole Moment for (B24N24)-Pt(Cl)2(NH3)2)	10.98 (Debye)	11.1 (Debye)

Basis set superposition Errors for complex: M062x /def2tzvp and M062x/gen/6-31G (d)//LanL2DZscfcyc = 5000 Counterpoise =2.

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Discussion

In this computational study, the same method Is used for the second base. The results show that changing the base series does not have much effect on the bond angle and bond length. Considering that not many changes were observed, then the basic series should be used, which consumes less time.

Although for the basis series 6-31G(d)//LanL2DZ, the dipole moment is slightly higher than the basis series Df2TZVP, but this value is not significant. The total electron energy for the complex is negative, indicating that the binding of chlorine to bromine is exothermic. The amount of energy released due to the bonding between chlorine and bromine is less than 10 kcal/mol, which Indicates physical absorption.

The amount of energy released for the two methods used is about 10% different, which is more negative for the Df2TZVP series.

Considering that in the synthesis of B24N24, carbon always appears in the structure, so it is suggested that the method of binding cisplatin on the boronitride sample doped with carbon should be investigated in future studies.

To answer the question whether B24N24 can be used to replace cisplatin, experimental and biological work should be done. In order to understand the real type of bond between Cl and Br, ELF theory of electron localization function as well as AIM theory should be used in future research.

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