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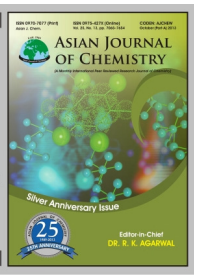

Thermodynamic Study Related to Antibiotic Attached to $B_5N_5C_8H_{18}$ nano Structure as a Nano Drug Carrier

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Density functional theory calculations were carried out to study the effects of binding penicillin and cefalexin to $B_5N_5C_8H_{18}$ nano structure. Binding energies, enthalpy, free Gibbs energy and entropy were calculated. Results from binding energies indicate that it is possible thermodynamically to covalently bind penicillin and cefalexin to $B_5N_5C_8H_{18}$ nano structure. The thermodynamic results show that the binding $B_5N_5C_8H_{18}$ nano structure to penicillin is easier than to cefalexin. The values of the HOMO, LUMO and HOMO-LUMO gap, for $B_5N_5C_8H_{18}$ nano structure, penicillin, cefalexin, $B_5N_5C_8H_{18}$/piniciline and $B_5N_5C_8H_{18}$/cefalexin were calculated. The value of HOMO-LUMO gap of $B_5N_5C_8H_{18}$ (0.15887) was decrease by attach to penicillin or cefalexin.

Key Words: Boron nitride, Pencillin, Cefalexin, Nano drug carrier.

INTRODUCTION

Due to excellent thermal and chemical stability, boron nitride ceramics are traditionally used as a part of high temperature equipment. Boron has a great potential in nanotechnology. The thermal conductivity of boron nitride is among the highest of all electric insulators. Little is known on the electronic structure and electro genetic behaviour of boron nitride in non bond interaction. Boron nitride has an isoelectronic feature and exists in various crystalline forms, including hexagonal and cubic forms. The hexagonal form corresponding to graphite is the most stable and softest one and is employed as the lubricant and additive to cosmetic product. The cubic form of BH_2NBH_2 analogous to diamond is called cubic boron nitride. The initial BH_2NBH_2 form is amorphous boron nitride powder and layer of amorphous boron nitride have been application in some semiconductor device. As diamond is less stable than graphite, cubic boron nitride is less stable than hexagonal boron nitride. the wurtzite form of boron nitride is hexagonal polymorph of carbon. In both cubic and wurtzite boron nitride, boron and nitrogen atoms are classified as tetrahedral, but the angle between neighboring tetrahedral are different[1-4]. The both hexagonal and cubic boron nitride are wide-gap semiconductors with the band gap energy corresponding to the UV region. If voltage is applied to hexagonal boron nitride or cubic boron nitride, it emits UV light in the range 215-250 nm and can employed as a light emitting diode or laser[5,6]. The physical properties and structural features of amorphous and crystalline boron nitride, graphite and diamond are as follows[1-8]. Due to isoelectronic characteristic of the non-carbon species $(BN)_n$ this compound can be consider as a limiting case of the B/N doped fullerenes and have become a subject of research intrest. This intreat may be linked to the fact that boron nitride has a stable crystalline phase similar to graphite[10-12]. The synthesis of C_{60} fulleren[13] followed by that of larger fullerene and carbon nanotubes raised the curtain on a new class of nano-objects based on layered material with predicted unique intrinsic physical properties[14]. The production of this novel graphite-like nanostructure opens up a new era in materials science and nano-scale engineering[15]. There has been a significant interest in experimental studies of B_nN_m clusters that can be found in the literature and several research groups have described the production of boron nitride-based nano structure[16-21]. Recently various cages and $(BN)_n$ cubes have been synthesized[22-27], boron nitride polyhedral have also been successfully synthesized by reaction of BCl_3 with NH_3 in laser beam[28,29]. There are mainly two structural classes for $(BN)_n$ cages[25,30,31]. In addition to the theoretical to predictions for the structure, physical properties of such molecules of $B_{24}C1_2N_{24}$ molecule[32] and $B_{12}N_{12}$, $B_{16}N_{16}$ and $B_{28}N_{28}$ molecule, the experimental synthesis and various spectrometer are needed for the final confirmation of their stability for structure[19,33]. However, there is basically no experimental and theoretical information on the $B_5N_5C_8H_{18}$ nano structure. So this paper focuses on the $B_5N_5C_8H_{18}$ nano structure as a new material for antibiotics carrier.

TABLE-1
CALCULATED THERMODYNAMIC PARAMETER FROM B3LYP LEVEL AND 6-311G** BASIS SET

	$B_5N_5C_8H_{18}$	Penicillin	Cefalexin	$B_5N_5C_8H_{18}$/Penicillin	$B_5N_5C_8H_{18}$/Cefalexin
ΔE (J/mol)	-1836546170	-3132668445	-4026873569	-5011448315	-5892536863
ΔH (J/mol)	-1836543691	-3132665972	-4026871093	-5011445839	-5892534387
ΔG (J/mol)	-1836704816	-3132764854	-4026970136	-5011719509	-5892778347
ΔS (J/Kmol)	540.688576	331.8207787	332.3576913	918.3581683	818.6596628

EXPERIMENTAL

Calculations on the isolated molecules and molecular complexes were performed within GAUSSIAN 03 package[34].

Antibiotic structure optimized with density functional theory using the 6-311G** basis set. Full geometry optimizations and frequency calculations were performed and each species was found to be a minimum by having no negative values in the frequency calculation. In order to obtain gas phase free energies at 298.15 K, it is necessary to calculate the zero-point energies and thermal corrections together with entropies to convert the internal energies to Gibbs energies at 298.15 K[35,36].

Frequency calculations on these structures verified that they were true minima and provided the necessary thermal corrections to calculate H (enthalpy) and G (Gibbs free energy). Finally, full optimizations and frequency calculations for each species were performed with the DFT/6-31G**[37-38].

In our model, penicillin and cefalexin was attached to $B_5N_5C_8H_{18}$ nano structure as an antibiotic carrier.

According to a charge analysis we determined the attaching site of antibiotics to the $B_5N_5C_8H_{18}$ nano structure[39].

The antibiotic/$B_5N_5C_8H_{18}$ nano structure was geometrically optimized using the 6-311G** basis set at the B3LYP level of theory. It is known that DFT methods give lower HOMO-LUMO gaps than HF methods and that is why we use a hybrid method B3LYP[40] for the calculation of the HOMO-LUMO gaps[41].

The HOMO-LUMO gaps were calculated using a hybrid DFT method that incorporates exact exchange using the GAUSSIAN 03 software[42].

The binding energies were calculated using the following equation[43]:

$$E_b = E(B_5N_5C_8H_{18}/X)-E(B_5N_5C_8H_{18})-E(X)$$

where $E(B_5N_5HC_8H_{18}/X)$ is the total electronic energy of the $B_5N_5HC_8H_{18}$ nano structure with attached antibiotic (penicillin or cefalexin, $E(B_5N_5HC_8H_{18})$ is the electronic energy of the $B_5N_5HC_8H_{18}$ nano structure and E(X) is the electronic energy of the antibiotic attached to the $B_5N_5HC_8H_{18}$ nano structure. Other binding parameters such as G_b, H_b and S_b calculated using the similar equation.

RESULTS AND DISCUSSION

Figs. 1 and 2 show optimized geometries of $B_5N_5HC_8H_{18}$ nano structure, $B_5N_5HC_8H_{18}$ nano structure/penicillin and $B_5N_5HC_8H_{18}$ nano structure/cefalexin.

Tables 1 and 2 display the values of the thermodynamic and binding parameter calculated for $B_5N_5HC_8H_{18}$ nano structure attached to antibiotic. The negative values of ΔH, ΔE and ΔG for $B_5N_5C_8H_{18}$ nano structure, penicillin, cefalexin, $B_5N_5C_8H_{18}$/piniciline and $B_5N_5C_8H_{18}$/cefalexin indicate that

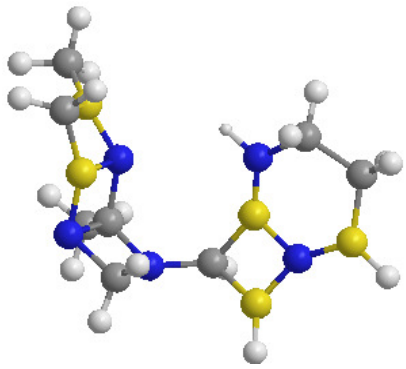

Fig. 1. Optimized $B_5N_5C_8H_{18}$ nano structure

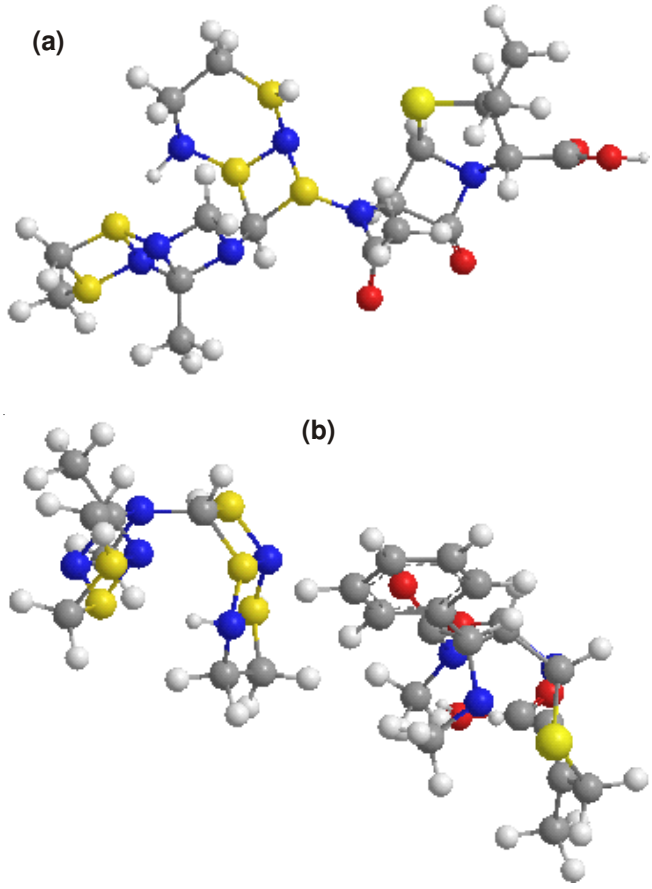

Fig. 2. Optimized a) $B_5N_5C_8H_{18}$ nano structure inside penicillin and b) $B_5N_5C_8H_{18}$ nano structure inside cefalexin

TABLE-2
BINDING PARAMETER CALCULATED FROM
B3LYP LEVEL AND 6-311G** BASIS SET

Binding Parameter	$B_5N_5C_8H_{18}$/Penicillin	$B_5N_5C_8H_{18}$/Cefalexin
ΔE_b (J/mol)	-42233699.59	-29117124.02
ΔH_b (J/mol)	-42236175.65	-29119602.7
ΔG_b (J/mol)	-42249838.6	-29103395.5
ΔS_b (J/Kmol)	45.84881393	-54.38660419

TABLE-3
CALCULATED HOMO, LUMO AND HOMO LUMO GAP ENERGIES FOR PENICILLIN, CEFALEXIN, $B_5N_5C_8H_{18}$, $B_5N_5C_8H_{18}$/PENICILLIN AND $B_5N_5C_8H_{18}$/CEFALEXIN AT 6-311G** BASIS SET

Descriptors	Penicillin	Cefalexin	$B_5N_5C_8H_{18}$	$B_5N_5C_8H_{18}$/Penicillin	$B_5N_5C_8H_{18}$/Cefalexin
HOMO (eV)	-0.26639	-0.24903	-0.19945	-0.18864	-0.19668
LUMO (eV)	-0.0337	-0.09036	-0.04058	-0.09307	-0.08801
HOMO–LUMO GAP (eV)	0.23269	0.15867	0.15887	0.09557	0.10867

these molecules are thermodynamically stable. Comparison of penicillin and cefalexin thermodynamic binding parameters indicate that binding $B_5N_5C_8H_{18}$ nano structure to penicillin easier than to cefalexin. The HOMO-LUMO gaps were calculated using a hybrid DFT method that incorporates exact exchange using the GAUSSIAN 03 software (Table-3)[44].

Table-3 displays the values of the HOMO, LUMO and HOMO-LUMO gap, for $B_5N_5C_8H_{18}$ nano structure, penicillin, cefalexin, $B_5N_5C_8H_{18}$/piniciline and $B_5N_5C_8H_{18}$/cefalexin. The $B_5N_5C_8H_{18}$ nano structure HOMO-LUMO gap value of 0.15887 decreasing by attach of penicillin or cefalexin.

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