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Density Functional Theory Study of B_6C_4Si Cluster as a Novel Drug Carrier

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ABSTRACT

The aim of the present study was to prepare new cluster (B_6C_4Si) as an antibiotic carrier. Density functional theory (DFT) method at the B3LYP level of theory in conjugate with the 6-311G** basis set was used to evaluate the interaction between B_6C_4Si cluster and Penicillin. Binding parameters, HOMO, LUMO and HOMO- LUMO GAP were calculated. Results show the B_6C_4Si HOMO–LUMO gap value of 0.13351 decreasing by attach of Penicillin. The negative values of ΔH_b, ΔE_b and ΔG_b indicate that B_6C_4Si /Penicillin are thermodynamically stable. From NMR shielding calculations, it can be seen that the penicillin connects stronger to B_6C_4Si cluster in positive charges than negative charge. Thus by creating positive field, penicillin can be connected to the B_6C_4Si cluster and delivered easily by using a negative filed.

Keywords: B_6C_4Si cluster, Drug carrier, Thermodynamic parameter, Penicillin

INTRODUCTION

Most studies have been performed on carbon nanotubes [1-3] and C_{60} [4], due to there have been discovered. Many novel structures such as carbon nanocones, and boron nitride nanocones have been viewed as intermediate between nanotubes and grapheme sheet [5, 6]. Because of their unique properties than those of carbon structure, more recently nanocones are more focused by scientist [7] and they believe these systems will revolutionized new future of nanoscience and technology and thus opening a very new and a vast filed of theoretical and experimental research. Studying the publications about nanocones beginning since 1994 [8], with employing various theoretical and experimental techniques to investigate properties of nanocones [9, 10], but most of these studies have been performed experimentally [11]. The fascinating novel structures of boron nitride (BN) [8] have been intensively studied, since they have unique and interesting properties such as electronic [12, 13] and mechanical properties [14-15]. Boron nanocones (BNNCs) represent an important class of nanocnes; consist of B and N atoms. The number of electrons in combination of B and N atoms is the same as two carbon atoms, therefore they have similar properties and also in some cases, they are

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better candidates to predict properties compare to other composite materials. BNNCs have been investigated and synthesized [8] and they have very interesting properties when compared with similar carbon nanostructure [16].
We have proposed a B_6C_4Si cluster as new carrier to attach to Penicillin, trough Si terminated atoms to investigate NMR shielding and thermodynamic properties.

COMPUTATIONAL DETAIL

In this study, density functional theory (DFT) calculation was used to optimize the molecular geometries of B_6C_4Si cluster, Penicillin and B_6C_4Si/Penicillin. Geometrical parameters were established and optimized. The optimized B_6C_4Si cluster, Penicillin and B_6C_4Si /Penicillin structures obtained from the Density Functional Theory B3LYP/6-311G** method (Figure 1 and 2).

It is known that DFT methods give lower HOMO–LUMO gaps than HF methods, and that is why we use a hybrid method B3LYP for the calculation of the HOMO–LUMO gaps [17]. The HOMO–LUMO gaps were calculated using a hybrid DFT method (Table 1) that incorporates exact exchange using the GAUSSIAN 03 software [18]. The binding energies were calculated using the following equation [19]:

$$\Delta E_b = E(B_6C_4Si / Penicillin) - E(B_6C_4Si) - E(Penicillin)$$

Where E (B_6C_4Si/X) is the total electronic energy of the B_6C_4Si cluster with the attached Penicillin, E(B_6C_4Si) is the electronic energy of the B_6C_4Si cluster, and E(X) is the electronic energy of the Penicillin. Also binding enthalpy, entropy and free Gibbs energy were calculated (Table 2).

Also the NMR isotropic shielding constants were calculated using the standard GIAO (Gauge-Independent Atomic Orbital) approach of Gaussian 03 program package. a) The isotropic value σ_{iso} of the shielding tensor which can be defined as:

$$\sigma_{iso} = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33})$$

b) The anisotropy parameter ($\Delta\sigma$) can be defined as:

If

$$|\sigma_{11} - \sigma_{iso}| \geq |\sigma_{33} - \sigma_{iso}| \quad \Delta\sigma = \sigma_{11} - \frac{\sigma_{22} + \sigma_{33}}{2}$$

If

$$|\sigma_{11} - \sigma_{iso}| \leq |\sigma_{33} - \sigma_{iso}| \quad \Delta\sigma = \sigma_{33} - \frac{\sigma_{22} + \sigma_{11}}{2}$$

and

c) The asymmetry parameter (η) is given by:

If

$$|\sigma_{11} - \sigma_{iso}| \geq |\sigma_{33} - \sigma_{iso}| \quad \eta = \frac{\sigma_{22} - \sigma_{33}}{\delta}$$

If

$$|\sigma_{11} - \sigma_{iso}| \leq |\sigma_{33} - \sigma_{iso}| \quad \eta = \frac{\sigma_{22} - \sigma_{11}}{\delta}$$

RESULT AND DISCUSSION

The HOMO–LUMO gaps were calculated using a hybrid DFT method that incorporates with exact exchange using the GAUSSIAN 03 software [18].
Table 1 displays the values of the HOMO, LUMO, and HOMO–LUMO gap, for B_6C_4Si cluster, Penicillin and B_6C_4Si /Penicillin. The B_6C_4Si cluster HOMO–LUMO gap value of 0.13351 decreasing by connecting of Penicillin. Table 2 displays the values of the binding parameters calculated for B_6C_4Si cluster attached to antibiotic. The negative values of ΔH_b, ΔE_b and ΔG_b indicate that

B_6C_4Si /Penicillin are thermodynamically stable.

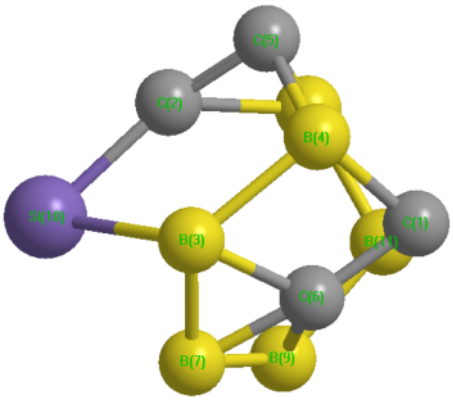


Fig. 1. The optimized structure of B_6C_4Si cluster.

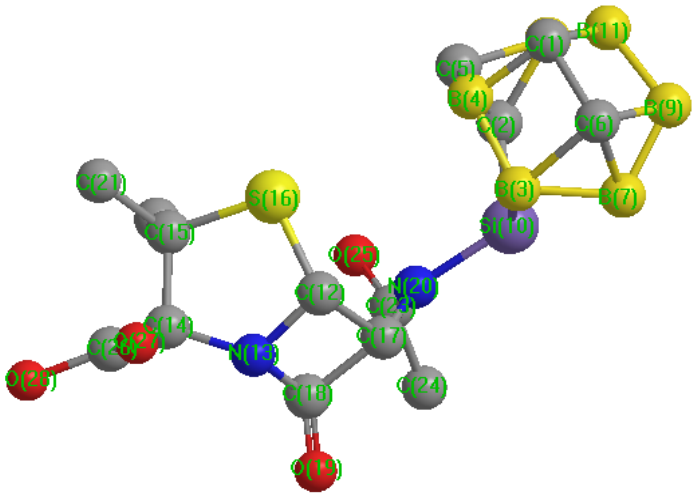


Fig. 2. The optimized B_6C_4Si cluster inside Penicillin.

Table 1. HOMO, LUMO and HOMO LUMO gap energy of Penicillin, B_6C_4Si and B_6C_4Si / Penicillin at 6-311G** basis set

Descriptors	**B_6C_4Si / Penicillin**	**B_6C_4Si**	**Penicillin**
HOMO(eV)	-0.26639	-0.24922	-0.23219
LUMO(eV)	-0.0337	-0.11571	-0.10561
HOMO-LUMO(eV)	0.23269	0.13351	0.12658

Table2. Binding parameter calculated from B3LYP level and 6-311G** basis set

Binding Parameter	**B_6C_4Si /Penicillin**
ΔE_b(kcal/mol)	-1521.761545
ΔH_b(kcal/mol)	-1523.538625
ΔG_b(kcal/mol)	-1516.751585
ΔS_b(kcal/Kmol)	-0.022775302

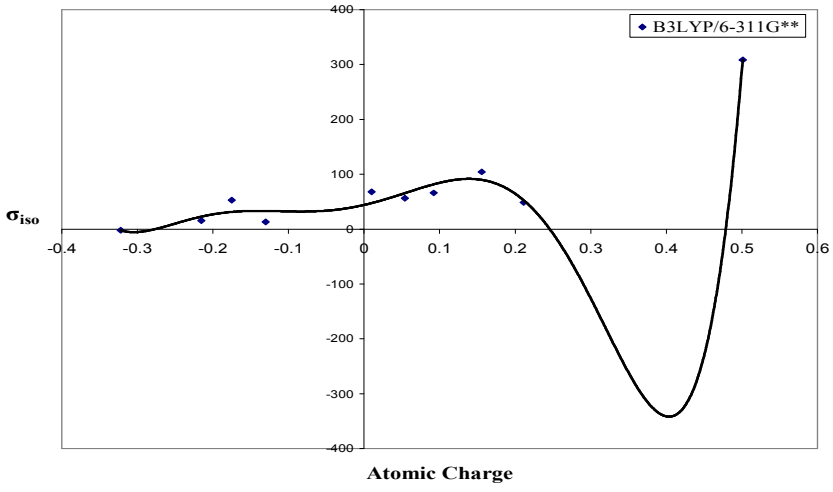
We studied B_6C_4Si cluster as a Penicillin carrier (Figure 1). Before and after connecting the Penicillin to B_6C_4Si, NMR calculations were performed in electric field of charges. NMR parameters are listed in Tables 4 to 5 in B3LYP level and 6-311G** basis set.

σiso, σaniso, Δσ, δ and η curves versus atomic charges for B_6C_4Si and B_6C_4Si /Penicillin are plotted in Figures 3 and 4. These curves are drawn for B3LYP level and 6-311G** set. These curves show that partial atomic charges have same behavior on the magnetic shielding of atoms and also show that the NMR System is very sensitive to partial atomic charges. Maximum points are around 0.4. So we can find that most chemical shielding is around 0.4. These curves show that the mechanism of positive charge is difference from negative charge. Positive and negative areas are different. Discussion on a σ_{aniso} and σ_{iso} curves are similar. There is a main different between σ_{aniso} and σ_{iso} curves. In a σ_{iso} curve minimum is around 0.4 but in σ_{aniso} curve maximum is around 0.4. This is also predictable and shows that these curves are very sensitive. δ and η are the results of σ_{iso} and σ_{aniso}. The minimum and maximum of σ_{iso} and σ_{aniso} curve shift to the 0.8 by connecting penicillin. Also δ and η curves have a similar behavior. The results show that penicillin to connect stronger to B_6C_4Si cluster in positive charges than negative charge. Thus by creating positive field, penicillin can be connected to the B_6C_4Si cluster and delivered easily by using a negative filed. So B_6C_4Si is good carrier for penicillin.

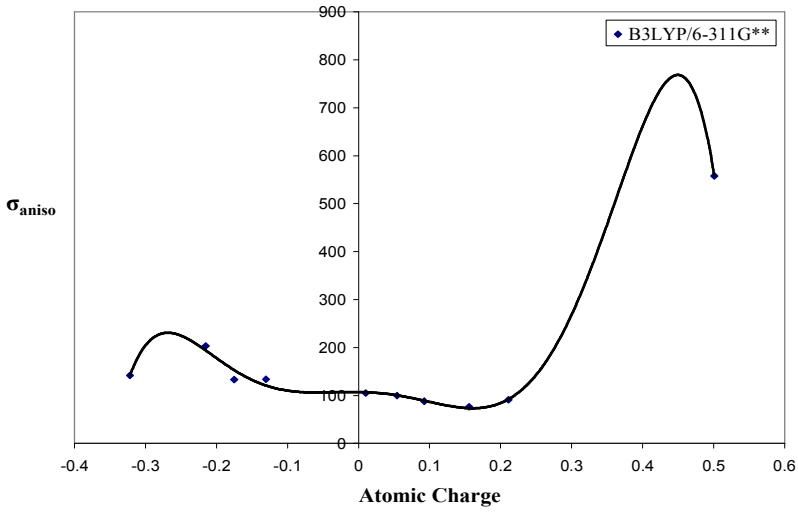
CONCLUSION

The interaction between penicillin and B_6C_4Si cluster have been investigated with density functional theory using B3LYP method and 6-311G** basis set. We analyzed the electronic structure and charge Mulliken population for the energetically most favorable complexes. Our results indicated that penicillin can form stable bindings with B_6C_4Si via the Si active site. Binding parameters, HOMO, LUMO and HOMO- LUMO GAP were calculated. Also the NMR shielding tensors have been investigated. The results show that penicillin connects stronger to B_6C_4Si cluster in positive charges than negative charge. Thus by creating positive field, penicillin can be connected to the B_6C_4Si cluster and delivered easily by using a negative filed. Thus, we arrive at the prediction that the B_6C_4Si can be implemented as a novel material for drug delivery applications.

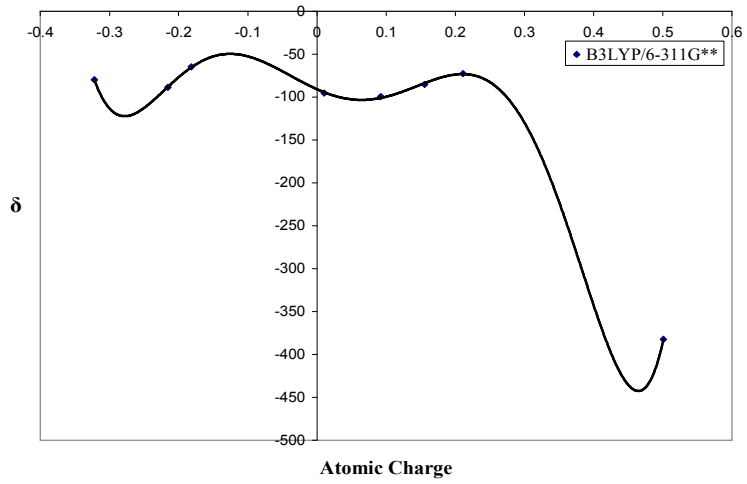
a)



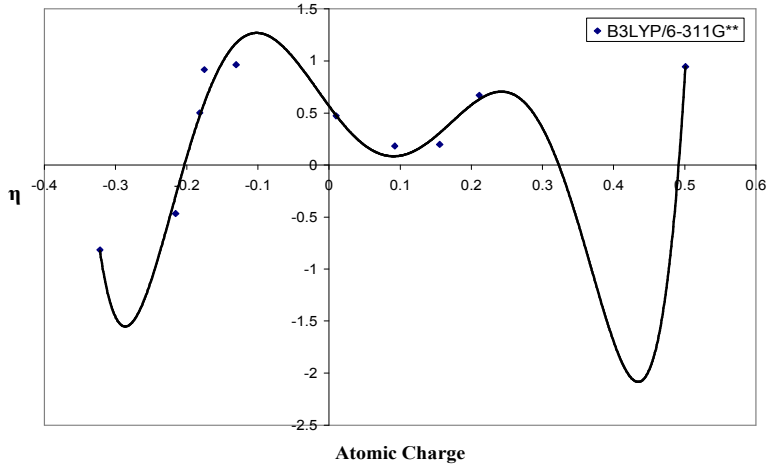
b)


B3LYP/6-311G**
σaniso
Atomic Charge

c)


B3LYP/6-311G**
δ
Atomic Charge

d)


B3LYP/6-311G**
η
Atomic Charge

e)

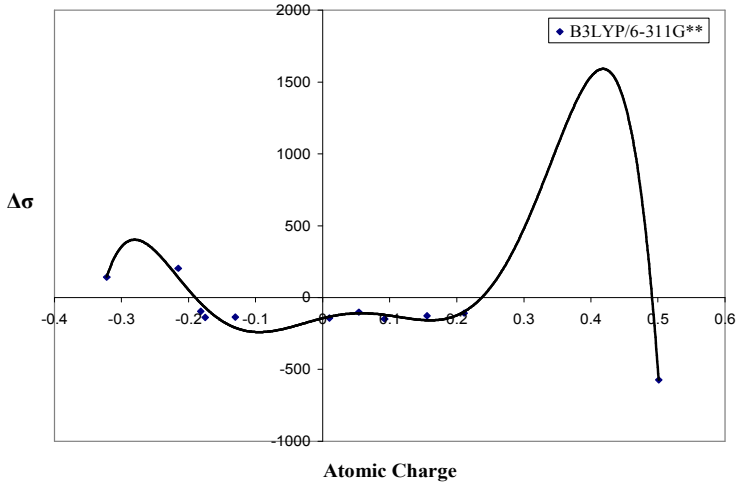
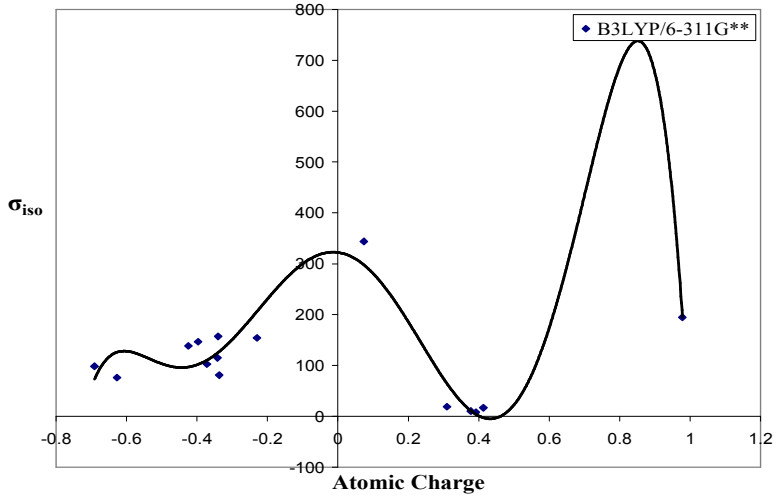
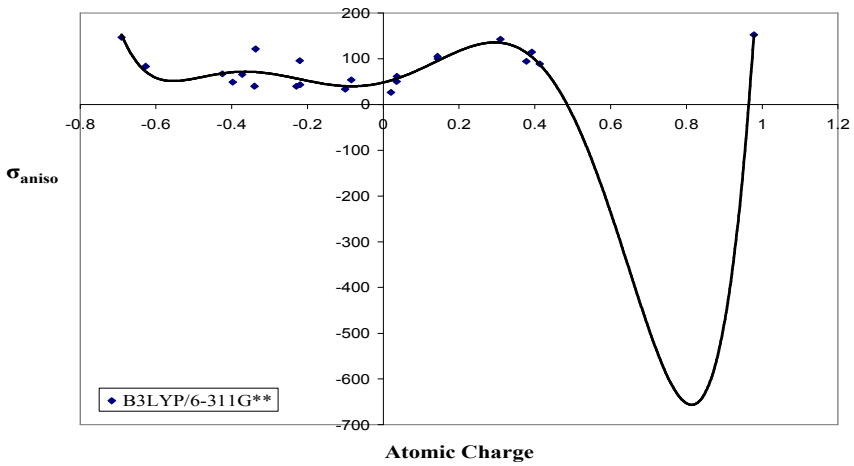


Fig. 3. Curve of a) σ_{iso} (ppm), b) σ_{aniso}(ppm), c) $\Delta\sigma$(ppm), d) δ(ppm) and e) η versus atomic charge for B_6C_4Si cluster.

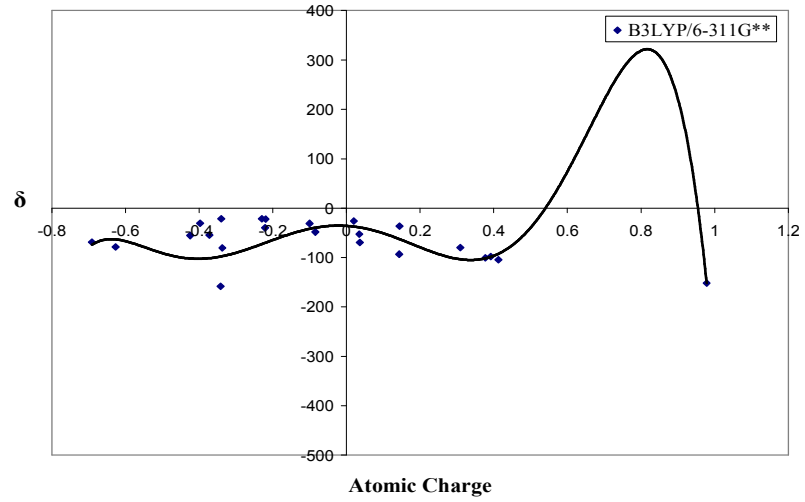
a)



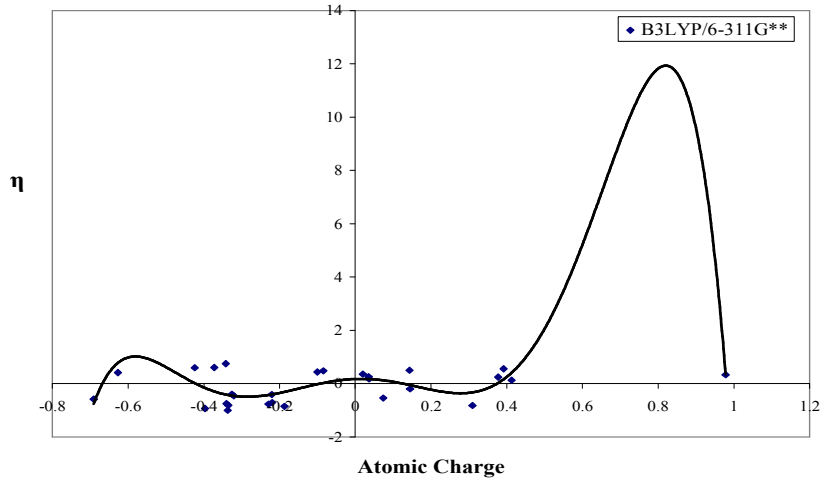
b)



c)



d)



e)

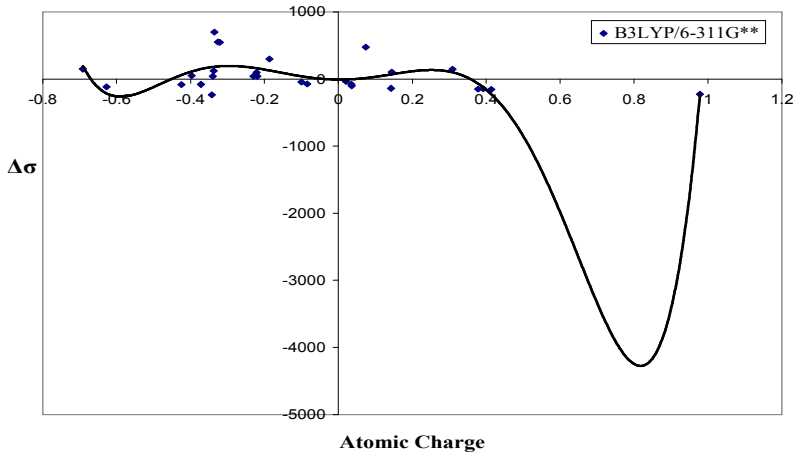


Fig. 4. Curve of a) σ_{iso}(ppm), b) σ_{aniso}(ppm), c) Δσ(ppm), d) δ(ppm), and e) η versus atomic charge for B_6C_4Si /Penicillin.

Table 3. List of calculation NMR Parameters for B_6C_4Si by B3LYP/6-311G** method.

Atom	Detminan (NMR)	ΔE(J)	δ(ppm)	η	Δσ(ppm)	Dipole Moment(D)	Atomic Charge
C (1)	324549.5925		-88.3601	-0.47	203.286		-0.215358
C (2)	91210.39027		-79.7009	-0.82	141.5942		-0.321866
B (3)	-297083.4761		-92.5767	0.92	-138.8651		-0.175145
B (4)	622371.3027		-85.1298	0.20	-127.6947		0.155613
C (5)	-31317.10107		-90.765	0.96	-136.14745		-0.130329
C (6)	-407968.0926	-1.5E+09	-99.1925	0.18	-148.78875	1.1104	0.092395
B (7)	766241.292		-64.5782	0.50	-96.86725		-0.181616
B (8)	-157207.8245		-72.671	0.67	-109.00645		0.211138
B (9)	384056.2708		-67.5724	0.97	-101.3585		0.053974
Si (10)	-16846750.47		-382.4966	0.95	-573.74485		0.501028
B (11)	-319285.5704		-95.1222	0.47	-142.6834		0.010166

Table 4. List of calculation NMR Parameters for B_6C_4Si/Penicillin by B3LYP/6-311G** method.

Atom	Detminan (NMR)	ΔE	δ(ppm)	η	Δσ(ppm)	Dipole Moment(D)	Atomic Charge
C (1)	3033368.717		-30.4481	-0.93	48.85		-0.397152
C (2)	422547.0239		-68.7821	-0.58	146.922		-0.690857
B (3)	-342258.4627		-93.1542	0.50	-139.73		0.143035
B (4)	426745.9574		-36.7699	-0.19	99.7747		0.144491
C (5)	2306111.88		-55.6915	0.60	-83.537		-0.424287
C (6)	2945357.158		-172.6675	-0.85	297.141		-0.186722
B (7)	159408.0577		-39.9708	-0.40	95.6749		-0.220684
B (8)	-30279.00586		-80.2989	-0.82	142.204		0.309268
B (9)	-157466.0201		-69.2395	0.18	-103.86		0.036259
Si (10)	9143775.882		-151.6397	0.34	-227.46		0.978172
B (11)	684718.5983		-52.6498	0.27	-78.975		0.035222
C (12)	937514.2403		-48.3091	0.48	-72.464		-0.084408
N (13)	299703.0466		-80.5478	-1.00	121.224		-0.337054
C (14)	1361018.085	-5E+09	-26.0177	0.36	-39.027	3.8485	0.020314
C (15)	807184.7651		-54.4682	0.60	-81.702		-0.372228
S (16)	21847496.05		-216.3163	-0.54	474.245		0.073878
C (17)	1281290.646		-30.9273	0.44	-46.391		-0.100247
C (18)	-405946.2365		-104.5761	0.13	-156.86		0.413104
O (19)	19436180.09		-234.9577	-0.45	545.292		-0.320945
N (20)	12502.67526		-78.5841	0.42	-117.88		-0.627016
C (21)	3563100.941		-21.5198	-0.77	39.8308		-0.229279
C (22)	3265769.374		-22.2767	-0.71	43.1639		-0.219663
C (23)	-217654.8291		-98.0186	0.56	-147.03		0.392063
C (24)	3779871.401		-21.3534	-0.75	40.1208		-0.340014
O (25)	42922219.32		-392.9545	-0.81	699.776		-0.335708
C (26)	-301614.5992		-100.5093	0.25	-150.76		0.377629
O (27)	20548744.43		-227.9737	-0.39	549.778		-0.32594
O (28)	-981550.5451		-158.249	0.75	-237.37		-0.341968

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