Journal of Physical and Theoretical Chemistry
of Islamic Azad University of Iran, 10 (1) 1-9: Spring 2013
(J. Phys. Theor. Chem. IAU Iran)
ISSN 1735-2126

NBO Analysis of Structural and Electronic Properties in $B_{30}N_{20}$

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Received September 2013; Accepted November 2013

ABSTRACT

In this paper, the structural properties of the $B_{30}N_{20}$ molecule have been investigated at B3LYP/6-31G (d) level of theory. The optimized structure and electronic properties calculations for the studied molecule have been performed using Gaussian 03 program. A mathematical equation of third degree was exploited for the correlation and exchange energy with the number of primitives. The Natural Bonding Orbital (NBO) analysis were performed on the $B_{30}N_{20}$ at the B3LYP/6-31G level of theory.

Keywords: DFT calculation; Boron-Nitride ($B_{30}N_{20}$); Primitive; NBO analysis; Exchange and correlation energy

INTRODUCTION

Since its discover by Iijima in 1991,carbon nanotubes (CNT) as a kind of quasi one-dimensional nanomaterial has been a hot subject of physical, chemical and material studies worldwide because of its unique functions in electro-conductivity and mechanics, and its potential applications in molecular devices and composite materials [1].

Beside carbon nanotubes, which are a promising material due to both their mechanical strength and their interesting electronic properties, boron nitride (BN) tubes have recently attracted increased attention.Considerable interest has been shown recently by boron nitride nanotubes (BNNTS)for application in nanoscale devices [2].

Boron nitride III-V is a compound known by marvelous chemical, optical, electrical, thermal and mechanical properties. Boron nitride is morphologically similar to a carbon system. Boron nitride acts like an electricity conductor and has good thermal conductivity properties. Boron nitride nanotube is similar to carbon nanotubes and has attracted more attention in nano electric and nano optic practices. Boron nitride nanotubes were first predicted theoretically [3, 4]. The first successful synthesis of boron nitride nanotubes was reported in 1995 [5].

In this paper, the structural properties of boron nitride with the formula of $B_{30}N_{20}$ are calculated by using the DFT methods

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with 6-21G(6D, 7F), 4-31G(6D, 7F), 6-31G(6D, 7F) AND 6-311G(6D,7F) basis sets. Then mathematical equations for correlation and exchange energies for this molecule have been calculated comparing to primitive numbers. The natural excess charge distribution and characterization of B-N bonds in $B_{30}N_{20}$ have been investigated by NBO.

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 nanostructures [2].

METHODS

All computational on $B_{30}N_{20}$ are carried out using Gaussian 03 program at the restricted LSDA, B3LYP, B3PW91, MPW1PW91, PBEPBE, PBE1PBE, B98, HCTH, HF, MP2 levels in 6-21g , 4-31g, 6-31g and 6-311g basis sets. Exchange and correlation energies in the above mentioned basis sets were calculated and the curve for correlation and exchange energies according to the number of primitives was drawn using Excel 2007 and the mathematical equation between them was obtained.

Energy minimum molecular geometries were located by minimizing energy.

Natural bonding orbital (NBO) analysis were performed on the $B_{30}N_{20}$ at the B3LYP/6-31G level of theory.

RESULTS AND DISCUSSION

Molecular properties

The structure of $B_{30}N_{20}$ is shown in figure 1. All computationals are carried out using Gaussian 03 program.

Theoretical calculation of bond lengthes for the B_{30}N20 was determined by optimizing the geometry (Table1).

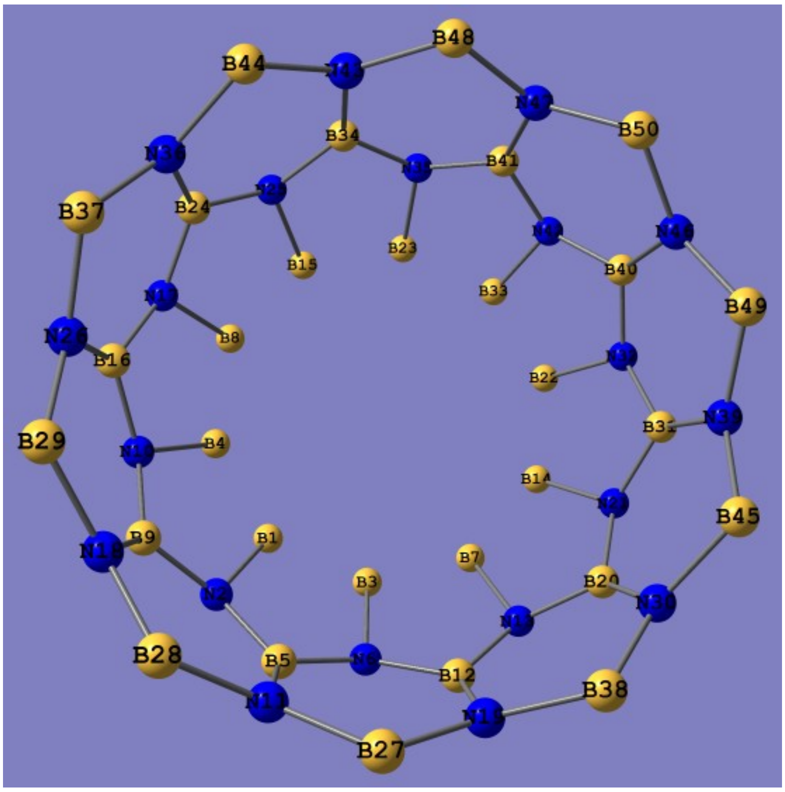

Fig. 1. The theoretical optimized possible geometric structure with numbering of $B_{30}N_{20}$**.**

Table 1. Calculated bond lengthes (A^0) for the $B_{30}N_{20}$

BOND	bond lengths (A^0)	BOND	bond lengths (A^0)
B1-N2	1.480900	B28-N18	1.478005
B3-N6	1.480758	B29-N18	1.477974
B4-N10	1.480787	B29-N26	1.478046
B5-N11	1.462247	B31-N21	1.445946
B5-N6	1.445943	B31-N32	1.446050
B5-N2	1.445971	B31-N39	1.462255
B7-N13	1.480816	B33-N42	1.480816
B8-N17	1.480809	B34-N25	1.446011
B9-N2	1.446062	B34-N35	1.446049
B9-N10	1.445935	B34-N43	1.462230
B9-N18	1.462238	B37-N26	1.478033
B12-N6	1.446110	B37-N36	1.478012
B12-N13	1.445952	B38-N19	1.477957
B12-N19	1.462206	B38-N30	1.478079
B14-N21	1.480862	B40-N32	1.445908
B15-N25	1.480746	B40-N42	1.446046
B16-N10	1.446103	B40-N46	1.462272
B16-N17	1.445934	B41-N35	1.445947
B16-N26	1.462264	B41-N42	1.445984
B20-N13	1.445975	B41-N47	1.462262
B20-N21	1.445958	B44-N36	1.477999
B20-N30	1.462191	B44-N43	1.477958
B22-N32	1.480835	B45-N30	1.478027
B23-N35	1.480837	B45-N39	1.477975
B24-N17	1.446045	B48-N43	1.477999
B24-N25	1.446055	B48-N47	1.478058
B24-N36	1.462245	B49-N39	1.478074
B27-N11	1.477994	B49-N46	1.477989
B27-N19	1.478108	B50-N46	1.478053
B28-N11	1.478100	B50-N47	1.477968

Exchange and Correlation Energy calculated:

The total optimized energy of $B_{30}N_{20}$ at the RHF and RMP2 levels in 6-21g, 4-31g, 6-31g and 6-311g basis sets were calculated using gussian 03. Correlation energies were calculated with equation 1. The results of these calculations are shown in tables 2 and 3 [6-9].

$$E_{correlation}=E_{RMP2} - E_{RHF} \qquad (1)$$

To calculate the exchange energy , total optimized energy of B30N20 at the restricted LSDA, B3LYP, B3PW91, MPW1PW91, PBEPBE, PBE1PBE, B98, HCTH, levels in the 6-21g, 4-31g, 6-31g and 6-311g basis sets are calculated. The average of energy differences at different levels is equal to exchange energies in the mentioned levels. The results of the exchange energy are shown in table 4.

The number of the primitives in 6-21G, 4-31G, 6-31g and 6-311g basis sets are 900, 1000, 1100, 1300 respectively. The correlation and exchange energies diagram in relation with the primitives number is drawn using Excel 2007 and using fitting method mathematical equations were exploited. The results are shown in the figures 2 and 3.

Table 2. The correlation energy calculated for $B_{30}N_{20}$ at 6-21G, 4-31G ,6-31G and 6-311G basis sets

Basis set	HF [a] (au)	MP2(au)	Ecorr.(au)=E(MP2)- E(HF)
6-21G	-1828.557162	-1828.557259	-9.658E-05
4-31G	-1828.602554	-1828.603101	-0.00054692
6-31G	-1829.549338	-1829.54978	-0.00044153
6-311G	-1830.038483	-1830.038491	-8.7E-06

a: atomic unit

Table 3. The primitive number and correlation energy calculated for B30N20 at 6-21G, 4-31G, 6-31G and 6-311G basis sets

Basis set	Primitive NO.	Ecorr. (au)
6-21G	900	-9.66E-05
4-31G	1000	-0.00054692
6-31G	1100	-0.00044153
6-311G	1300	-8.70E-06

Table 4. The exchange energy calculated for B30N20 at 6-21G ,4-31G ,6-31G and 6-311G basis set

	total energy (au)				energy difference (au)			
method	6-21g	4-31g	6-31g	6-311g	6-21g	4-31g	6-31g	6-311g
LSDA	-1828.87963	-1828.104607	-1830.012873	-1830.608861	10.89636418	10.86950467	10.90539593	10.82249292
B3LYP	-1839.775995	-1838.974112	-1840.918269	-1841.431354				
B3PW91	-1838.963881	-1838.146713	-1840.095117	-1840.57373	0.81211383	0.82739859	0.82315142	0.85762418
B3LYP	-1839.775995	-1838.974112	-1840.918269	-1841.431354				
B3PW91	-1838.963881	-1838.146713	-1840.095117	-1840.57373	0.31094776	0.30152159	0.30333197	0.30059036
MPW1PW91	-1839.274828	-1838.448235	-1840.398449	-1840.87432				
MPW1PW91	-1839.274828	-1838.448235	-1840.398449	-1840.87432	0.50116607	0.525877	0.51981945	0.55703382
B3LYP	-1839.775995	-1838.974112	-1840.918269	-1841.431354				
PBEPBE	-1837.443131	-1836.650191	-1838.604179	-1838.604179	0.1123036	0.07048096	0.06570937	0.53951835
PBE1PBE	-1837.555435	-1836.720672	-1838.669888	-1839.143697				
B98	-1839.149445	-1838.329238	-1840.274894	-1840.762752	0.62654924	0.64487388	0.64337483	0.66860195
B3LYP	-1839.775995	-1838.974112	-1840.918269	-1841.431354				
PBEPBE	-1837.443131	-1836.650191	-1838.604179	-1839.094833	2.33286332	2.32392079	2.3140896	2.33652114
B3LYP	-1839.775995	-1838.974112	-1840.918269	-1841.431354				
PBE1PBE	-1837.555435	-1836.720672	-1838.669888	-1839.143697	2.22055972	2.25343983	2.24838023	2.28765681
B3LYP	-1839.775995	-1838.974112	-1840.918269	-1841.431354				
HCTH	-1839.128733	-1838.383833	-1840.309467	-1840.785536	0.64726146	0.59027865	0.60880179	0.6458177
B3LYP	-1839.775995	-1838.974112	-1840.918269	-1841.431354				
		average			**2.0511**	**2.0453**	**2.0480**	**2.1129**

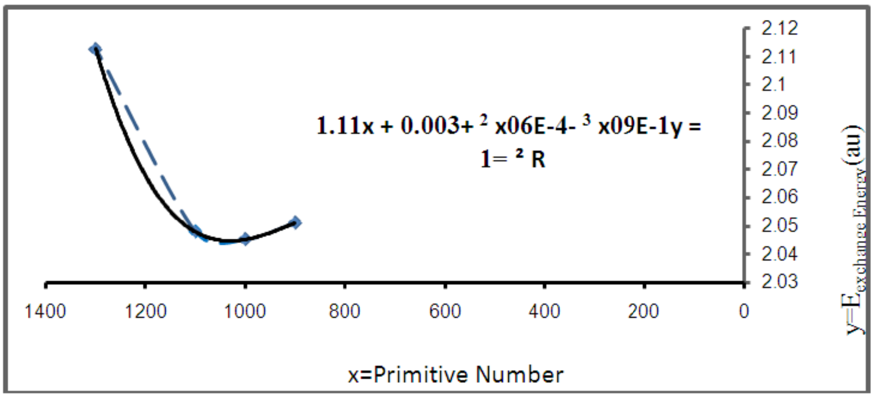

Fig.2 . The exchange energy of the $B_{30}N_{20}$ system as a primitive number at different levels of theory with 6-21 G, 4-31G, 6-31G and 6-311G basis sets.
(— — — — — Calculated data, ———————fitted)

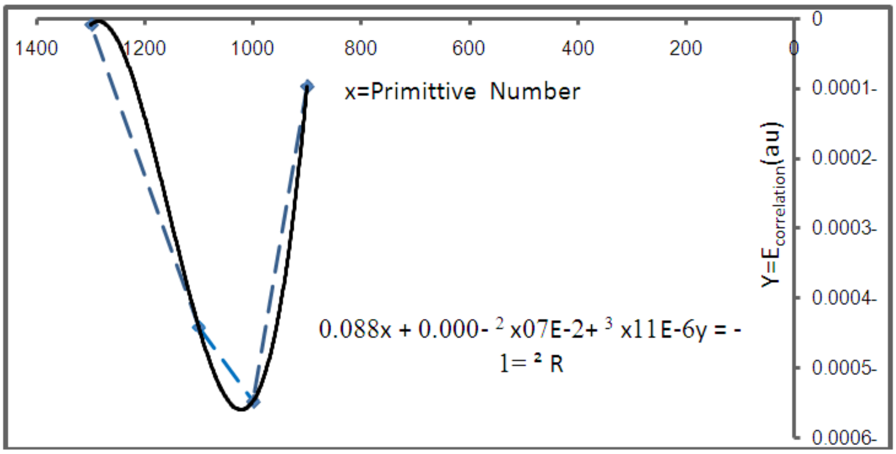

Fig. 3. The correlation energy of the $B_{30}N_{20}$ system as a primittive number at different levels of theory with 6-21G, 4-31G, 6-31G and 6-311G basis sets.
(— — — — — Calculated data, ———— fitted)

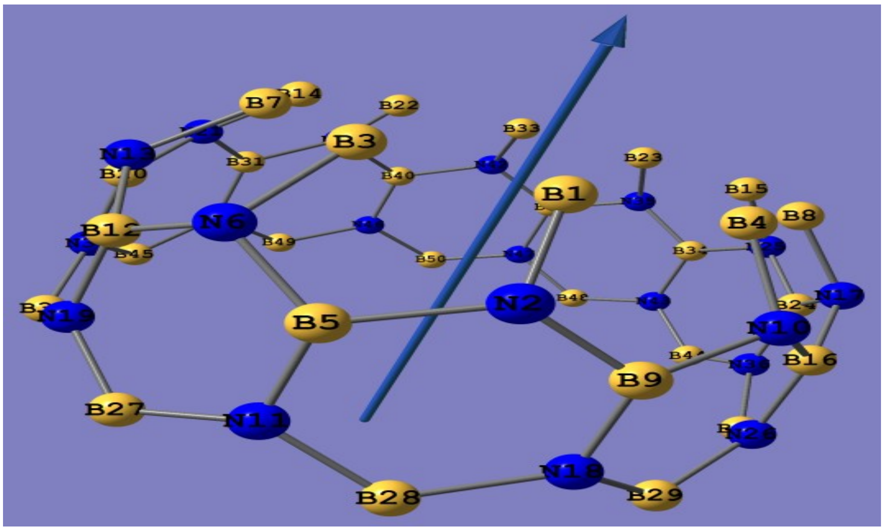

Fig. 4. The direction of dipole moment of the B30N20.

NBO study on the structure of the $B_{30}N_{20}$

Among the theoretical methods, natural bond orbital (NBO) is a special one to evaluate atom charges. NBO calculation was carried out using Gaussian 03 program at the B3LYP/6-31G level [10, 11].

It is clear that in this structure, Boron and Nitrogen atoms have positive and negative charges respectively. The natural charge on the boron atoms at both ends of the molecule are less than the other boron atoms. The natural charge on the internal boron atoms are more and about +0.7. The natural charge on the nitrogen atoms at the end of the molecule are more than the inner nitrogen atoms in the molecule and are -0.79 and -0.75 one by one.

Hybridization studies on the atoms in the structure of $B_{30}N_{20}$ shows that S% is between 22.9 to 38.55. Internal boron atoms have Hybridization level of SP^2. Also S% of the boron atoms is between 38.55 to 22.9 and for nitrogen it is between 31.13 to 37.15. S% for the boron atoms decreases in the direction of dipole moment which is shown in figure 4.The results of NBO are shown in table 5.

Table 5. NBO analysis of the $B_{30}N_{20}$ at the B3LYP/6-31G level theory

BOND	NBO analysis	BOND	NBO analysis
BD (1) B 1 - N 2	0.4578* (sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 1 - N 2	0.8890*(sp 3.37)B -0.4578*(sp 2.02)N
BD (2) B 1 - N 2	0.3185* (sp99.99)B+ 0.9479* (sp99.99)N	BD*(2) B 1 - N 2	0.9479*(sp99.99)B-0.3185*(sp99.99)N
BD (1) B 1 - B 3	0.7071* (sp 1.60)B+ 0.7071* (sp 1.60)B	BD*(1) B 1 - B 3	0.7071*(sp 1.60)B -0.7071*(sp 1.60)B
BD (1) B 1 - B 4	0.7071* (sp 1.59)B+ 0.7071* (sp 1.59)B	BD*(1) B 1 - B 4	0.7071* (sp 1.59)B -0.7071*(sp 1.59)B
BD (1) N 2 - B 5	0.8770* (sp 2.00)N+0.4805* (sp 1.99)B	BD*(1) N 2 - B 5	0.4805* (sp 2.00)N -0.8770*(sp 1.99)B
BD (1) N 2 - B 9	0.8777* (sp 1.98)N+ 0.4793* (sp 2.03)B	BD*(1) N 2 - B 9	0.4793* (sp 1.98)N -0.8777*(sp 2.03)B
BD (1) B 3 - N 6	0.4579* (sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 3 - N 6	0.8890*(sp 3.37)B -0.4579*(sp 2.02)N
BD (2) B 3 - N 6	0.3184* (sp99.99)B+ 0.9480* (sp99.99)N	BD*(2) B 3 - N 6	0.9480*(sp99.99) -0.3184* (sp99.99)N
BD (1) B 3 - B 7	0.7071* (sp 1.59)B+ 0.7071* (sp 1.59)B	BD*(1) B 3 - B 7	0.7071* (sp 1.59)B-0.7071* (sp 1.59)B
BD (1) B 4 - B 8	0.7071* (sp 1.60)B+ 0.7071* (sp 1.60)B	BD*(1) B 4 - B 8	0.7071* (sp 1.60)B-0.7071* (sp 1.60)B
BD (1) B 4 - N 10	0.4579* (sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 4 - N 10	0.8890* (sp 3.37)B-0.4579*(sp 2.02)N
BD (2) B 4 - N 10	0.3185*(sp99.99)B+ 0.9479* (sp99.99)N	BD*(2) B 4 - N 10	0.9479*(sp99.99)B -0.3185*(sp99.99)N
BD (1) B 5 - N 6	0.4805* (sp 1.99)B+ 0.8770* (sp 2.00)N	BD*(1) B 5 - N 6	0.8770*(sp 1.99)B -0.4805*(sp 2.00)N
BD (1) B 5 - N 11	0.4752*(sp 2.03)B+ 0.8799*(sp 1.70)N	BD*(1) B 5 - N 11	0.8799*(sp 2.03)B-0.4752*(sp 1.70)N
BD (2) B 5 - N 11	0.2983* (sp99.99)B+ 0.9545* (sp99.99)N	BD*(2) B 5 - N 11	0.9545*(sp99.99)B -0.2983*(sp99.99)N
BD (1) N 6 - B 12	0.8776* (sp 1.98)N+ 0.4793* (sp 2.03)B	BD*(1) N 6 - B 12	0.4793*(sp 1.98)N -0.8776* (sp 2.03)B
BD (1) B 7 - N 13	0.4578*(sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 7 - N 13	0.8890*(sp 3.37)B-0.4578*(sp 2.02)N
BD (2) B 7 - N 13	0.3184*(sp99.99)B+ 0.9480* (sp99.99)N	BD*(2) B 7 - N 13	0.9480*(sp99.99)B -0.3184*(sp99.99
BD (1) B 7 - B 14	0.7071* (sp 1.60)B+ 0.7071* (sp 1.60)B	BD*(1) B 7 - B 14	0.7071* (sp 1.60)B-0.7071* (sp 1.60)B
BD (1) B 8 - B 15	0.7071* (sp 1.59)B+ 0.7071* (sp 1.59)B	BD*(1) B 8 - B 15	0.7071* (sp 1.59)B-0.7071* (sp 1.59)B
BD (1) B 8 - N 17	0.4579* (sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 8 - N 17	0.8890*(sp 3.37)B-0.4579*(sp 2.02)N
BD (2) B 8 - N 17	0.3184*(sp99.99)B+ 0.9480* (sp99.99)N	BD*(1) B 8 - N 17	0.9480*(sp99.99)B -0.3184*(sp99.99)N
BD (1) B 9 - N 10	0.4793* (sp 2.03)B+ 0.8776*(sp 1.98)N	BD*(1) B 9 - N 10	0.8776*(sp 2.03)B-0.4793*(sp 1.98)N
BD (1) B 9 - N 18	0.4806*(sp 1.94)B+ 0.8769* (sp 1.90)N	BD*(1) B 9 - N 18	0.8769*(sp 1.94)B -0.4806*(sp 1.90)N
BD (2) B 9 - N 18	0.3016* (sp99.99)B+ 0.9534* (sp1.00)N	BD*(2) B 9 - N 18	0.9534*(sp99.99)B-0.4806*(sp 1.90)N
BD (1) N 10 - B 16	0.8769*(sp 2.00)N+0.4806* (sp2.02)B	BD*(1) N 10 - B 16	0.4806* (sp 2.00)N -0.8769*(sp 2.02)B
BD (1) N 11 - B 27	0.8935*(sp 2.19)N+0.4491* (sp 1.60)B	BD*(1) N 11 - B 27	0.4491*(sp 2.19)N -0.8935*(sp 1.60)B
BD (1) N 11 - B 28	0.8935*(sp 2.19)N+0.4491* (sp 1.60)B	BD*(1) N 11 - B 28	0.4491*(sp 2.19)N -0.8935*(sp 1.60)B
BD (1) B 12 - N 13	0.4793*(sp 2.03)B+ 0.8776*(sp 1.98)N	BD*(1) B 12 - N 13	0.8776*(sp 2.03)B-0.4793*(sp 1.98)N
BD (1) B 12 - N 19	0.4806*(sp 1.94)B+ 0.8769* (sp 1.90)N	BD*(1) B 12 - N 19	0.8769*(sp 1.94)B -0.4806*(sp 1.90)N
BD (2) B 12 - N 19	0.3017* (sp99.99)B+ 0.9534* (sp1.00)N	BD*(2) B 12 - N 19	0.9534*(sp99.99)B-0.3017*(sp 1.00)N
BD (1) N 13 - B 20	0.8769*(sp 2.00)N+0.4806* (sp2.02)B	BD*(1) N 13 - B 20	0.4806* (sp 2.00)N -0.8769*(sp 2.02)B
BD (1) B 14 - N 21	0.4579* (sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 14 - N 21	0.8890*(sp 3.37)B-0.4579*(sp 2.02)N
BD (2) B 14 - N 21	0.3184* (sp99.99)B+ 0.9480* (sp99.99)N	BD*(2) B 14 - N 21	0.9480*(sp99.99)B -0.3184*(sp99.99)N
BD (1) B 14 - B 22	0.7071* (sp 1.59)B+ 0.7071* (sp 1.59)B	BD*(1) B 14 - B 22	0.7071* (sp 1.59)B-0.7071* (sp 1.59)B
BD (1) B 15 - B 23	0.7071* (sp 1.60)B+ 0.7071* (sp 1.60)B	BD*(1) B 15 - B 23	0.7071* (sp 1.60)B-0.7071* (sp 1.60)B
BD (1) B 15 - N 25	0.4578*(sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 15 - N 25	0.8890*(sp 3.37)B-0.4578*(sp 2.02)N
BD (2) B 15 - N 25	0.3183* (sp99.99)B+ 0.9480* (sp99.99)N	BD*(2) B 15 - N 25	0.9480*(sp99.99)B -0.3183*(sp99.99)N
BD (1) B 16 - N 17	0.4806*(sp 2.02)B+ 0.8769*(sp2.00)N	BD*(1) B 16 - N 17	0.8769*(sp 2.02)B -0.4806*(sp 2.00)N
BD (1) B 16 - N 26	0.4753*(sp 2.02)B+ 0.8798*(sp1.98)N	BD*(1) B 16 - N 26	0.8798*(sp 2.02)B -0.4753*(sp1.69)N

Table 5. Continued

BD (1) N 17 - B 24	0.8776*(sp 1.98)N+ 0.4793* (sp 2.03)B	BD*(1) N 17 - B 24	0.4793* (sp 1.98)N -0.8776*(sp 2.03)B
BD (1) N 18 - B 28	0.8949*(sp 2.05)N+0.4464* (sp 1.87)B	BD*(1) N 18 - B 28	0.4464*(sp 2.05)N -0.8949* (sp 1.87)B
BD (1) N 18 - B 29	0.8948*(sp 2.05)N+0.4464* (sp 1.87)B	BD*(1) N 18 - B 29	0.4464*(sp 2.05)N -0.8948* (sp 1.87)B
BD (1) N 19 - B 27	0.8949*(sp 2.05)N+0.4463* (sp 1.87)B	BD*(1) N 19 - B 27	0.4463*(sp 2.05)N -0.8949* (sp 1.87)B
BD (1) N 19 - B 38	0.8949* (sp 2.05)N+0.4464* (sp 1.87)B	BD*(1) N 19 - B 38	0.4464*(sp 2.05)N -0.8949* (sp 1.87)B
BD (1) B 20 - N 21	0.4806*(sp 2.02)B+ 0.8769*(sp2.00)N	BD*(1) B 20 - N 21	0.8769*(sp 2.02)B -0.4806*(sp 2.00)N
BD (1) B 20 - N 30	0.4753* (sp 2.02)B+ 0.8798*(sp1.69)N	BD*(1) B 20 - N 30	0.8798*(sp 2.02)B -0.4753*(sp1.69)N
BD (1) N 21 - B 31	0.8776*(sp 1.98)N+ 0.4793* (sp 2.03)B	BD*(1) N 21 - B 31	0.4793* (sp 1.98)N -0.8776*(sp 2.03)B
BD (1) B 22 - N 32	0.4579*(sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 22 - N 32	0.8890*(sp 3.37)B-0.4579*(sp 2.02)N
BD (2) B 22 - N 32	0.3185*(sp99.99)B+ 0.9479* (sp99.99)N	BD*(2) B 22 - N 32	0.9479*(sp99.99)B-0.3185*(sp99.99)N
BD (1) B 22 - B 33	0.7071* (sp 1.60)B+ 0.7071* (sp 1.60)B	BD*(1) B 22 - B 33	0.7071* (sp 1.60)B-0.7071* (sp 1.60)B
BD (1) B 23 - B 33	0.7071* (sp 1.59)B+ 0.7071* (sp 1.59)B	BD*(1) B 23 - B 33	0.7071* (sp 1.59)B-0.7071* (sp 1.59)B
BD (1) B 23 - N 35	0.4579*(sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 23 - N 35	0.8890*(sp 3.37)B-0.4579*(sp 2.02)N
BD (2) B 23 - N 35	0.3184*(sp99.99)B+ 0.9480* (sp99.99)N	BD*(2) B 23 - N 35	0.9480*(sp99.99)B -0.3184*(sp99.99)N
BD (1) B 24 - N 25	0.4793*(sp 2.03)B+ 0.8776*(sp 1.98)N	BD*(1) B 24 - N 25	0.8776*(sp 2.03)B-0.4793*(sp 1.98)N
BD (1) B 24 - N 36	0.4806*(sp 1.94)B+ 0.8769* (sp 1.91)N	BD*(1) B 24 - N 36	0.8769*(sp 1.94)B -0.4806*(sp 1.91)N
BD (2) B 24 - N 36	0.3016*(sp99.99)B+ 0.9534* (sp1.00)N	BD*(2) B 24 - N 36	0.9534*(sp99.99)B-0.3016*(sp 1.00)N
BD (1) N 25 - B 34	0.8769*(sp 2.00)N+0.4806* (sp2.02)B	BD*(1) N 25 - B 34	0.4806* (sp 2.00)N -0.8769*(sp 2.02)B
BD (1) N 26 - B 29	0.8935*(sp 2.21)N+ 0.4490*(sp 1.60)B	BD*(1) N 26 - B 29	0.4490*(sp 2.21)N -0.8935*(sp 1.60)B
BD (2) N 26 - B 29	0.9565*(sp99.99)N+ 0.2918* (sp99.99)B	BD*(2) N 26 - B 29	0.2918*(sp99.99)N-0.9565*(sp99.99)B
BD (1) N 26 - B 37	0.8935*(sp 2.21)N+ 0.4490*(sp 1.60)B	BD*(1) N 26 - B 37	0.4490*(sp 2.21)N -0.8935*(sp 1.60)B
BD (1) B 27 - B 38	0.7091*(sp 2.70)B+ 0.7051*(sp 2.65)B	BD*(1) B 27 - B 38	0.7051*(sp 2.70)B -0.7091*(sp 2.65)B
BD (1) B 28 - B 29	0.7091*(sp 2.70)B+ 0.7051*(sp 2.65)B	BD*(1) B 28 - B 29	0.7051*(sp 2.70)B -0.7091*(sp 2.65)B
BD (1) N 30 - B 38	0.8935*(sp 2.21)N+ 0.4490*(sp 1.60)B	BD*(1) N 30 - B 38	0.4490*(sp 2.21)N -0.8935*(sp 1.60)B
BD (2) N 30 - B 38	0.9565*(sp99.99)N+ 0.2918* (sp99.99)B	BD*(2) N 30 - B 38	0.2918*(sp99.99)N-0.9565*(sp99.99)B
BD (1) N 30 - B 45	0.8935*(sp 2.21)N+ 0.4490*(sp 1.60)B	BD*(1) N 30 - B 45	0.4490*(sp 2.21)N -0.8935*(sp 1.60)B
BD (1) B 31 - N 32	0.4793*(sp 2.03)B+ 0.8776*(sp 1.98)N	BD*(1) B 31 - N 32	0.8776*(sp 2.03)B-0.4793*(sp 1.98)N
BD (1) B 31 - N 39	0.4806*(sp 1.94)B+ 0.8769* (sp 1.90)N	BD*(1) B 31 - N 39	0.8769*(sp 1.94)B -0.4806*(sp 1.90)N
BD (2) B 31 - N 39	0.3016*(sp99.99)B+ 0.9534* (sp1.00)N	BD*(2) B 31 - N 39	0.9534*(sp99.99)B-0.3016*(sp 1.00)N
BD (1) N 32 - B 40	0.8769*(sp 2.00)N+0.4806* (sp2.02)B	BD*(1) N 32 - B 40	0.4806* (sp 2.00)N -0.8769*(sp 2.02)B
BD (1) B 33 - N 42	0.4578* (sp 3.37)B+ 0.8890*(sp 2.02)N	BD*(1) B 33 - N 42	0.8890*(sp 3.37)B-0.4578*(sp 2.02)N
BD (2) B 33 - N 42	0.3185*(sp99.99)B+ 0.9479* (sp99.99)N	BD*(2) B 33 - N 42	0.9479*(sp99.99)B-0.3185*(sp99.99)N
BD (1) B 34 - N 35	0.4806*(sp 2.02)B+ 0.8769*(sp2.00)N	BD*(1) B 34 - N 35	0.8769*(sp 2.02)B -0.4806*(sp 2.00)N
BD (1) B 34 - N 43	0.4753*(sp 2.02)B+ 0.8798*(sp1.69)N	BD*(1) B 34 - N 43	0.8798*(sp 2.02)B -0.4753*(sp1.69)N
BD (1) N 35 - B 41	0.8776*(sp 1.98)N+ 0.4793* (sp 2.03)B	BD*(1) N 35 - B 41	0.4793* (sp 1.98)N -0.8776*(sp 2.03)B
BD (1) N 36 - B 37	0.8949* (sp 2.05)N+0.4464* (sp 1.87)B	BD*(1) N 36 - B 37	0.4464*(sp 2.05)N -0.8949* (sp 1.87)B
BD (1) N 36 - B 44	0.8949* (sp 2.05)N+0.4464* (sp 1.87)B	BD*(1) N 36 - B 44	0.4464*(sp 2.05)N -0.8949* (sp 1.87)B
BD (1) B 37 - B 44	0.7071* (sp 2.70)B+ 0.7071* (sp 1.69)B	BD*(1) B 37 - B 44	0.7071*(sp 2.70)B -0.7071*(sp 2.69)B
BD (1) N 39 - B 45	0.8949* (sp 2.05)N+0.4463* (sp 1.87)B	BD*(1) N 39 - B 45	0.4463*(sp 2.05)N -0.8949* (sp 1.87)B
BD (1) N 39 - B 49	0.8948*(sp 2.05)N+0.4464* (sp 1.87)B	BD*(1) N 39 - B 49	0.4464*(sp 2.05)N -0.8948* (sp 1.87)B
BD (1) B 40 - N 42	0.4806*(sp 2.02)B+ 0.8769*(sp2.00)N	BD*(1) B 40 - N 42	0.8769*(sp 2.02)B -0.4806*(sp 2.00)N
BD (1) B 40 - N 46	0.4753*(sp 2.02)B+ 0.8798*(sp1.69)N	BD*(1) B 40 - N 46	0.8798*(sp 2.02)B -0.4753*(sp1.69)N
BD (1) B 41 - N 42	0.4793*(sp 2.03)B+ 0.8776*(sp 1.98)N	BD*(1) B 41 - N 42	0.8776*(sp 2.03)B-0.4793*(sp 1.98)N
BD (1) B 41 - N 47	0.4806* (sp 1.94)B+0.8769(sp 1.90)N	BD*(1) B 41 - N 47	0.8769*(sp 1.94)B -0.4806*(sp 1.90)N

Table 5. Continued

BD (2) B 41 - N 47	0.3016*(sp99.99)B+ 0.9535* (sp1.00)N	BD*(2) B 41 - N 47	0.9534*(sp99.99)B-0.3016*(sp 1.00)N
BD (1) N 43 - B 44	0.8935* (sp 2.21)N+0.4490*(sp 1.60)B	BD*(1) N 43 - B 44	0.4490*(sp 2.21)N -0.8935*(sp 1.60)B
BD (1) N 43 - B 48	0.8935*(sp 2.21)N+0.4490*(sp 1.60)B	BD*(1) N 43 - B 48	0.4490*(sp 2.21)N -0.8935*(sp 1.60)B
BD (2) N 43 - B 48	0.9565*(sp99.99)N+ 0.2918* (sp99.99)B	BD*(2) N 43 - B 48	0.2918*(sp99.99)N-0.9565*(sp99.99)B
BD (1) B 45 - B 49	0.7091*(sp 2.70)B+ 0.7051*(sp 2.65)B	BD*(1) B 45 - B 49	0.7051*(sp 2.70)B -0.7091*(sp 2.65)B
BD (1) N 46 - B 49	0.8935*(sp 2.21)N+ 0.4490*(sp 1.60)B	BD*(1) N 46 - B 49	0.4490*(sp 2.21)N -0.8935*(sp 1.60)B
BD (2) N 46 - B 49	0.9565*(sp99.99)N+ 0.2919* (sp99.99)B	BD*(2) N 46 - B 49	0.2918*(sp99.99)N-0.9565*(sp99.99)B
BD (1) N 46 - B 50	0.8935*(sp 2.21)N+ 0.4490*(sp 1.60)B	BD*(1) N 46 - B 50	0.4490*(sp 2.21)N -0.8935*(sp 1.60)B
BD (1) N 47 - B 48	0.8948*(sp 2.05)N+0.4464* (sp 1.87)B	BD*(1) N 47 - B 48	0.4464*(sp 2.05)N -0.8948* (sp 1.87)B
BD (1) N 47 - B 50	0.8949* (sp 2.05)N+0.4464* (sp 1.87)B	BD*(1) N 47 - B 50	0.4464*(sp 2.05)N -0.8948* (sp 1.87)B
BD (1) B 48 - B 50	0.7052*(sp 2.65)B+ 0.7090*(sp 2.70)B	BD*(1) B 48 - B 50	0.7090*(sp 2.65)B -0.7052*(sp 2.709)B

Table 6. Global chemical reactivity indices for $B_{30}N_{20}$ at the level of B3LYP/6-31 G theory

	B3LYP/6-31g
E total /hartree	-1840.918
E HOMO/ev	-4.555
E LUMO/ev	-3.663
E gap/ev	0.892
Dipole moment / (Debye)	4.7402

Frontier molecular orbital

Both the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are the main orbital which take part in chemical stability. The HOMO represents the ability to donate an electron, LUMO as an electron acceptor represents the ability to obtain an electron. The HOMO and LUMO energies were calculated by B3LYP/ 6-31G method. Energy difference between HOMO and LUMO orbital is called as energy gap which is an important stability for structures. The large LUMO-HOMO gap is often concerned as a molecule stability condition. The HOMO–LUMO energies and energy gap were also calculated at the B3LYP/6-31G and the values are listed in table 6.

CONCLUSION

DFT calculations are carried out using Gaussian 03 program. The structure of the molecule $B_{30}N_{20}$ is totally optimized. A mathematical equation of third degree was exploited for the correlation and exchange energy with the number of primitives. Regarding the NBO analysis S% decreases in the direction of dipol moment for the boron atoms. S% is in the range of 22.9 to 38.55 for boron nitride. Internal boron atoms use SP^2 hybridization.

The electronic properties, E gap and dipole moment are calculated using B3LYP/6-31g and the values of these are 0.892 (ev) and 4.7402 Debye respectively. Therefore $B_{30}N_{20}$ shows poor conductivity.

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