International Scholars Journals

International Journal of Diseases and Disorders ISSN 2329-9835 Vol. 6 (3), pp. 001-014, March, 2018. Available online at www.internationalscholarsjournals.org © International Scholars Journals

Full Length Research Paper

Density functional theory (DFT) based study of solvent effect on $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$ nano structures

M. Monajjemi[1]*, S. Mohajeri[1] and F. Mollaamin[2]

[1]Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran.
[2]Department of Chemistry, Qom Branch, Islamic Azad University, Qom, Iran.

Accepted 15 July, 2017

In this present work, all calculations were carried out with the Gaussian 98 program based on density functional theory (DFT) at B3LYP/3-21G level of theory. Then stability and grand state of $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$ nanocones in bulk and different solvents were investigated. It is clear that solvent effects were reviewed with concentration on quantitative values of Gibbs free energy, enthalpy, internal energy and dipole moment in the spread of solvents around these two nano structures and temperature effect was studied on the stability of these novel structures in the same solvents. Furthermore we compared the results of gas phase and different solvents when surrounding these two nano structures. In this work, NMR shielding parameters were calculated based on each atom to recognize active sites in these two systems. The results showed that because of high stability of $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$, these novel structures could be the best candidates and most favorable in biological systems and drug delivery.

Key words: Density functional theory (DFT), solvent effect, optimized molecule, nanocone, nuclear magnetic resonance (NMR) investigation, Gauge including atomic orbital (GIAO), drug delivery.

INTRODUCTION

Since C60 (Kroto et al., 1985) and carbon nanotubes (CNTs) (Iijima, 1991; Iijima and Ichihashi, 1993; Bethune, 1993) have been discovered, these structures have been used in different studies and scientists have been guided by this new information to find the best results about these novel structures. The studies about nanocones have been performed since 1994, (Rubio et al., 1994) and we have been able to obtain a great deal of information about properties of these systems but most of these results have been computed experimentally (Bourgeois et al., 2000; Sachdeva et al., 2010). An important group of nanocones is Boron nitride nanocones (BNNCs) and these curved structures and carbon nanocones have more fascinating properties than other nano structures. A complete analogy between C and BN structures is not possible, since, for instance, a pentagonal ring made by B and N atoms will introduce at least one homonuclear bond (Machado et al., 2003).

*Corresponding author. E-mail: m_monajjemi@yahoo.com.

Then, in general, the situation, concerning electronic and structural properties, is less focused for BN than for C cones (Machado et al., 2003). Taking into account the chemical and mechanical stability of nanocones and little tip degradation, BNNCs can be applied as good candidates for field emitters (Machado et al., 2003).

BN clusters (Oku et al., 2003) and BNNCs are made of B and N atoms therefore we can see that there is a negative charge at nitrogen atom and a positive charge at boron atom, in addition these negative and positive charges and unique properties such as reactivity and polarity show that we can apply an electrophilic or nucleophilic reagent as a solution for these structures (Oku et al., 2003).

Recently BNNCs particles have been synthesizes (Rubio et al., 1994; Bourgeois et al., 2000; Terauchi et al., 2000). Also studies of these novel systems show that they are built of conical shells and these structures are seamless (Bourgeois et al., 2000).These novel structures are applicable in various and different fields. Most of the researches about carbon structures have been redone with these nanocones (Charlier and Rignanese, 2001). A

comparison between these novel systems and CNTs has led to the understanding that BNNCs have more interesting characteristics than the CNTs (Nirmala and Kolandaivel, 2007; Mollaamin et al., 2011).

Moreover, theoretical investigations on $(BN)_n$ nanocones have been performed in vast fields and show that they are better candidates than CNTs when there is not any experimental result (Kroto et al., 1985; Bourgeois et al., 2000). Thus the scientists have more focused on these novel researches (Iijima et al., 1992) because these structures can open a vast field of nanoscience both theoretically and experimentally.

In the present study, we address the relative stability and NMR parameters for two kinds of BNNCs, $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$ in spread of solvents and temperatures. The results were compared to find the best solvent and temperature.

METHODOLOGY

The Gaussian 98 program was applied to obtain the best prediction of these structures in the electronic grand state (Monajjemi et al., 2008). This program was used to study many specific properties of $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$ such as thermodynamic properties, Atomic charges, Multipole moment and NMR shielding in gas phase and different solvenst and temperatures. The instrument used in this survey of the geometric structure optimization and computing properties of $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$ nanocones was density functional theory (DFT). The DFT method used in this study was Becke 3 Lee-Yang-Parr (B3LYP) (Becke, 1993; Becke, 1992; Becke, 1992) functional. The B3LYP functional is selected since it seems to give a better description of dispersion interactions, and hence, of the physical adsorption among all presently available functional. Primary basis sets describe the atomic orbitals and also shows the best description of the electronic structures.B3LYP method with split valence basis set (3-21G) was used in this study. So geometry optimizations in the gas phase and different solvents and temperatures [19-23] for $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$ were done at B3LYP/3-21G level of theory (Becke, 1993; Becke, 1992).

Frequency analyses were used to show that the optimized structures are true minima and wave function is ground state, without imaginary frequencies (Monajjemi et al., 2010; Mollaamin et al., 2008).

The interaction between the solute and the solvent molecules has a crucial role in clarifying various molecular processes involved in chemistry. The optimized molecule in the gas phase was applied as an initial input for subsequent B3LYP/3-21G level of theory calculations to simulate the solvent effect. In both of these structures, temperatures were changed from 298 to 320K respectively. Solvent effects on $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$ were reviewed in different solvents and six different temperatures of 298, 300, 305, 310, 315 and 320 K by using the same method and basis set. Finally the best solvent and temperature for these structures were reported.

Environmental effects and also the structure of molecule widely revolutionize NMR spectroscopy thus we can calculate NMR parameters to predict influence of solvent effect (Monajjemi et al., 2007; Monajjemi et al., 2008). Atoms in various solvents can experience different amount of shielding because of this reason we can recognize the active sites of these structures (Monajjemi et al., 2008). On the other hand an NMR calculation can play an important role in understanding the function of a biomolecule such as Glycine. All of the NMR shielding (De Dios et al., 1999) tensors are calculated in the basis of gauge-including atomic orbital (GAIO) method at B3LYP/3-21G level of theory not only $B_{10}N_{11}$ but also $B_{10}N_{11}H_7$ $(Gly)_2$ and the position of active sites are recognized for these two structures.

RESULTS AND DISCUSSION

In the present study, interaction of $B_{10}N_{11}$ nanocone with two Glycine molecules is considered. All calculations were performed to study the relative stability of $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$ especially thermodynamic properties and NMR shielding tensors in different solvents and temperatures.

We selected a particular nanocone as $B_{10}N_{11}$ in this study. $B_{10}N_{11}$ nanocone was optimized in gas phase and different solvents and temperatures with B3LYP/3-21G level of theory. The optimization structure has been carried out to find ground state structure shown in Figure 1. As follow two molecules of Glycine (Amino Acid) were stuck to $B_{10}N_{11}$ nanocone through boron terminated atoms. Thus two molecules of Glycine were only weakly adsorbed on pristine $B_{10}N_{11}$ by van der Waals (vdW) interaction. Finally the top and bottom dangling bonds were saturated by hydrogen atoms. The optimization structures of $B_{10}N_{11}H_7$ $(Gly)_2$ have been shown in Figure 2. Then stability of this novel structures in gas phase and the same solvents and temperatures were reviewed and to this case thermodynamic parameters were considered at B3LYP/3-21G level of theory. Thermodynamic parameters, which were computed in gas phase and different solvents and temperatures, were containing internal energy (E), enthalpy (H), Gibbs free energy (G) and entropy(S). These results are shown in Tables 1 and 2. Figure 3 shows thermodynamic parameters in different solvents and temperatures for $B_{10}N_{11}$ nanocone. In the end these results for $B_{10}N_{11}$ nanocone and $B_{10}N_{11}H_7$ $(Gly)_2$ were compared and the best solvent and temperature for these structures were selected.

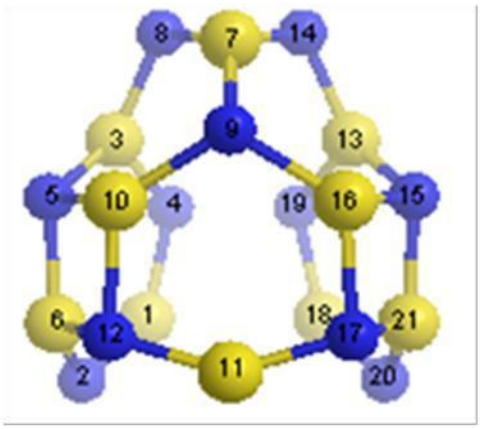
Then NMR parameters were applied for recognizing active sites of $B_{10}N_{11}$ nanocone and $B_{10}N_{11}H_7$ $(Gly)_2$ in gas phase and different solvents. These results are summarized in Tables 3, 4 and 5. Also Figures 4 and 5 indicate NMR parameters for these two structures respectively.

Average Mulliken charge values per atom for these structures are reported in Tables 6 and 7. Also the values of dipole moments (Debye) for these two structures in gas phase and different solvents are given in Table 8.

In general all calculations on $B_{10}N_{11}$ nanocone and $B_{10}N_{11}H_7$ $(Gly)_2$ have been done in gas phase and different solvents and temperatures in B3LYP/3-21G level of theory.

Conclusion

Primarily the study of various molecules in different dielectric constants is the most prevalent investigation of computational chemistry. Firstly, in the present study, we



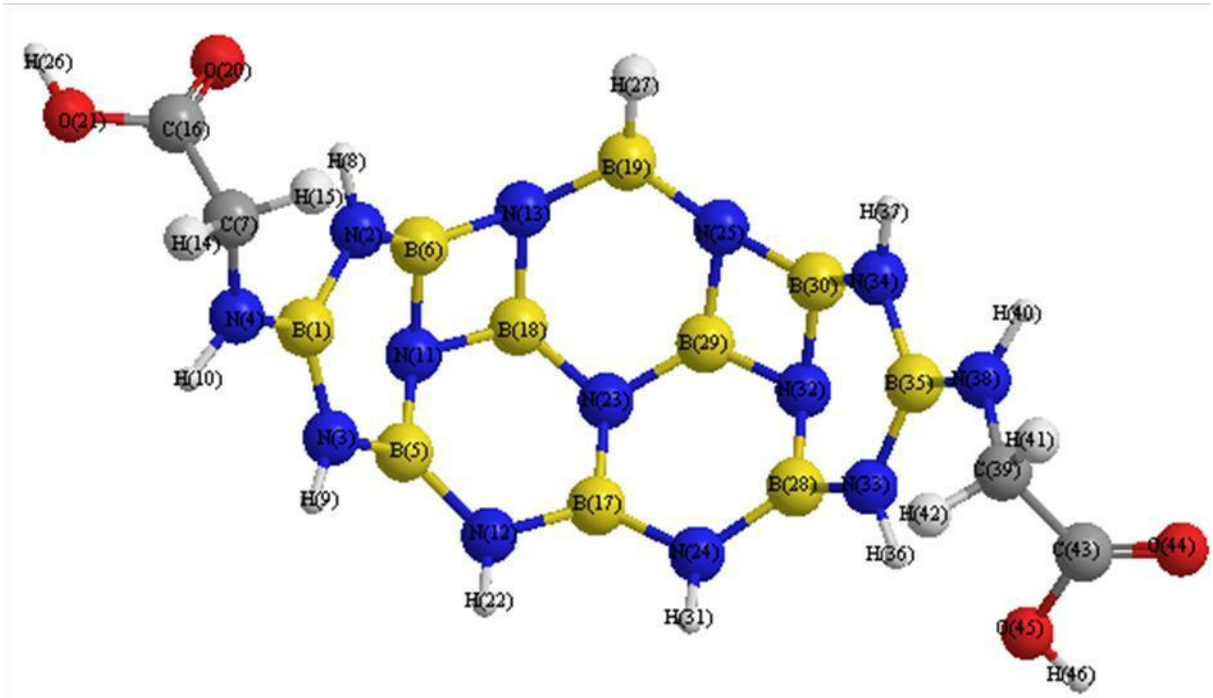


Figure 1. The optimization structure for $B_{10}N_{11}$ nanocone.

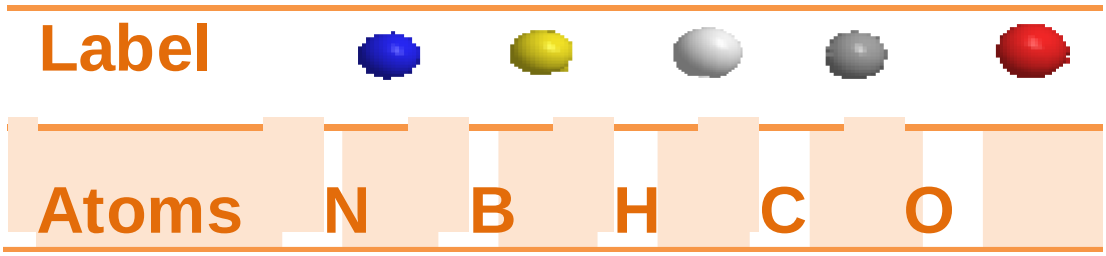


Figure 2. The optimization structure and pictorial view for $B_{10}N_{11}H_7$ (Gly) $_2$ in B3LYP/3-21G level of theory. The blue, yellow, white, gray and red balls indicate nitrogen, boron, hydrogen, carbon and oxygen atoms, respectively.

Table 1. Thermodynamic parameters for $B_{10}N_{11}$ in gas phase and different solvents and temperatures (internal energy, Gibbs free energy, enthalpy and entropy) in B3LYP/3-21G level of theory.

Temperature			298K	310K	312K	313K	315K	320K
Phase	Gas ε=1	-G(Kcal/mol)	531112.6396	531113.8877	531114.1004	531114.2077	531114.4217	531114.9607
		-H(Kcal/mol)	531081.5666	531080.8945	531080.7790	531080.7207	531080.6033	531080.3084
		-E(Kcal/mol)	531082.1589	531081.5107	531081.3990	531081.3425	531081.2296	531080.9441
		S(cal/mol.K)	104.219	106.428	106.801	106.987	107.360	108.290
	Water ε=78.39	-G(Kcal/mol)	531112.5285	531113.7754	531113.9881	531114.0948	531114.3094	531114.8478
		-H(Kcal/mol)	531081.4888	531080.8179	531080.7025	531080.6441	531080.5274	531080.2319
		-E(Kcal/mol)	531082.0817	531081.4342	531081.3225	531081.2660	531081.1530	531080.8681
		S(cal/mol.K)	104.107	106.314	106.686	106.872	107.244	108.174
	Ethanol ε=24.55	-G(Kcal/mol)	531112.5379	531113.7848	531113.9981	531114.1048	531114.3188	531114.8578
		-H(Kcal/mol)	531081.4963	531080.8248	531080.7094	531080.6510	531080.5343	531080.2388
		-E(Kcal/mol)	531082.0887	531081.4411	531081.3294	531081.2729	531081.1600	531080.8750
		S(cal/mol.K)	104.116	106.323	106.695	106.881	107.253	108.183
	Methanol ε=32.63	-G(Kcal/mol)	531112.5348	531113.7816	531113.9950	531114.1017	531114.3157	531114.8541
		-H(Kcal/mol)	531081.4950	531080.8236	531080.7081	531080.6498	531080.5331	531080.2381
		-E(Kcal/mol)	531082.0874	531081.4398	531081.3281	531081.1593	531081.1593	531080.8738
		S(cal/mol.K)	104.109	106.316	106.688	106.874	107.246	108.176
	DMSO ε=46.8	-G(Kcal/mol)	531112.5310	531113.7779	531113.9906	531114.0973	531114.3113	531114.8503
		-H(Kcal/mol)	531081.4906	531080.8192	531080.7037	531080.6454	531080.5287	531080.2337
		-E(Kcal/mol)	531082.0830	531081.4354	531081.3237	531081.2679	531081.1549	531080.8694
		S(cal/mol.K)	104.110	106.317	106.689	106.875	107.247	108.175
	Benzene ε=2.247	-G(Kcal/mol)	531112.6145	531113.8620	531114.0753	531114.1820	531114.3960	531114.9350
		-H(Kcal/mol)	531081.5534	531080.8820	531080.7659	531080.7081	531080.5908	531080.2959
		-E(Kcal/mol)	531082.1458	531081.4982	531081.3865	531081.3300	531081.2170	531080.9315
		S(cal/mol.K)	104.178	106.387	106.759	106.945	107.318	108.248
	Cyclohexane ε=2.023	-G(Kcal/mol)	531112.6182	531113.8664	531114.0791	531114.1864	531114.4004	531114.9394
		-H(Kcal/mol)	531081.5565	531080.8845	531080.7690	531080.7106	531080.5939	531080.2984
		-E(Kcal/mol)	531082.1489	531081.5007	531081.3890	531081.3325	531081.2196	531080.9340
		S(cal/mol.K)	104.183	106.392	106.765	106.951	107.323	108.253

Table 2. Thermodynamic parameters for $B_{10}N_{11}H_7$ (Gly) $_2$ in different solvents and temperatures (internal energy, Gibbs free energy, enthalpy and entropy) in B3LYP/3-21G level of theory.

Temperature			298K	310K	312K	313K	315K	320K
Phase	Gas ε=1	-G(Kcal/mol)	888298.6756	888300.7721	888301.1304	888301.3105	888301.6713	888302.5787
		-H(Kcal/mol)	888246.5534	888245.2971	888245.0813	888244.9727	888244.7543	888244.2034
		-E(Kcal/mol)	888247.1458	888245.9138	888245.7013	888245.5946	888245.3800	888244.8397
		S(cal/mol.K)	174.819	178.950	179.646	179.993	180.688	182.423
	Water ε=78.39	-G(Kcal/mol)	888298.8444	888300.9886	888301.3551	888301.5389	888301.9079	888302.8354
		-H(Kcal/mol)	888245.5174	888244.2630	888244.0471	888243.9386	888243.7208	888243.0450
		-E(Kcal/mol)	888246.1104	888244.8792	888244.6671	888244.5604	888244.3471	888243.8068
		S(cal/mol.K)	178.859	182.984	183.679	184.026	184.720	186.453
	Methanol ε=32.63	-G(Kcal/mol)	888298.6091	888300.7414	888301.1060	888301.2886	888301.6557	888302.5787
		-H(Kcal/mol)	888245.5758	888244.3214	888244.1055	888243.9969	888243.7792	888243.2289
		-E(Kcal/mol)	888246.1681	888244.9376	888244.7255	888244.6188	888244.4048	888243.8645
		S(cal/mol.K)	177.874	182.000	182.694	183.041	183.735	185.468

Table 2. Contd.

DMSO ε=46.8	-G(Kcal/mol)	888298.6913	888300.8280	888301.1938	888301.3770	888301.7441	888302.6691
	-H(Kcal/mol)	888245.5450	888244.2900	888244.0741	888243.9656	888243.7478	888243.1981
	-E(Kcal/mol)	888246.1374	888244.9062	888244.6941	888244.5881	888244.3741	888243.8338
	S(cal/mol.K)	178.254	182.380	183.075	183.422	184.116	185.848
Benzene ε=2.247	-G(Kcal/mol)	888298.8187	888300.9265	888301.2873	888301.4680	888301.8307	888302.7438
	-H(Kcal/mol)	888246.3940	888245.1384	888244.9219	888244.8133	888244.5956	888244.0446
	-E(Kcal/mol)	888246.9864	888245.7546	888245.5419	888245.4352	888245.2212	888244.6809
	S(cal/mol.K)	175.834	179.963	180.658	181.006	181.700	183.434
Cyclohexane ε=2.023	-G(Kcal/mol)	888298.7842	888300.8888	888301.2490	888301.4298	888301.7918	888302.7036
	-H(Kcal/mol)	888246.4392	888245.1836	888244.9677	888244.8591	888244.6408	888244.0904
	-E(Kcal/mol)	888247.0322	888245.7998	888245.5877	888245.4810	888245.2670	888244.7261
	S(cal/mol.K)	175.565	179.694	180.389	180.737	181.431	183.165

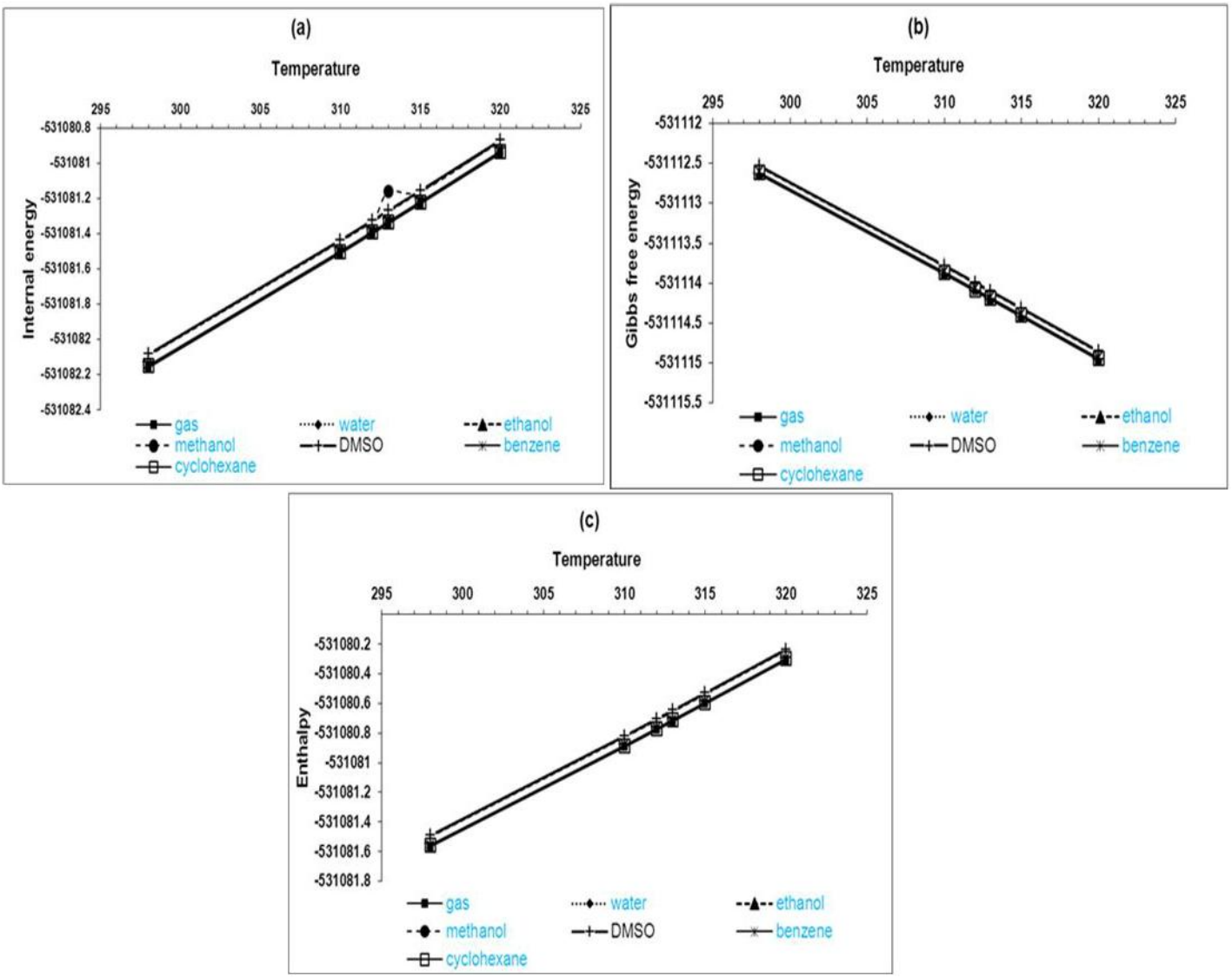


Figure 3. The values of thermodynamic parameters of $B_{10}N_{11}$ nanocone (in different solvents and temperatures)(a) Internal energy, (b) Gibbs free energy, (c)Enthalpy in B3LYP/3-21G level of theory.

Table 3. NMR parameters for $B_{10}N_{11}$ in different solvents and B3LYP/3-21G level of theory.

Atom	Gas phase										
	2N	**5N**	**8N**	**9N**	**11B**	**12N**	**14N**	**17N**	**18B**	**20N**	**21B**
σ_{iso}	-2.2376	91.3121	59.158	154.1968	95.4365	157.414	59.1592	157.4146	88.1406	-2.24	98.3552
σ_{aniso}	164.9609	115.7558	190.4065	159.8339	114.3935	103.5578	190.4056	103.5584	66.643	164.9617	47.4759
$\Delta\sigma$	164.961	115.7557	190.4065	159.8189	114.3936	103.5579	590.4057	103.5584	66.643	164.9616	-62.43235
η	0.91366805	0.5975366	0.7551279	0.2821943	0.3283282	0.162076	0.7551197	0.1620796	0.8773743	0.9137554	0.5208762
δ	109.974	77.1705	126.9377	106.556	76.2624	69.0386	126.9371	69.0389	44.4287	109.9744	-41.6216
ε=78.39						**Water**					
σ_{iso}	-3.6244	90.8872	60.2257	153.2421	95.4071	157.7798	60.2262	157.78	88.289	-3.6243	98.2333
σ_{aniso}	166.1689	116.1077	190.3351	160.5471	113.3632	104.2296	190.3344	104.2303	66.3397	166.1671	47.186
$\Delta\sigma$	166.1689	116.10765	190.33505	160.54715	113.36315	104.22965	190.3344	104.23035	66.3397	166.1671	-62.5592
η	0.936642495	0.607356621	0.733462841	0.290016761	0.32995525	0.173236221	0.733665053	0.173242726	0.879922399	0.936688749	0.50852513
δ	110.7793	77.4051	126.89	107.0314	75.5754	69.4872	126.8538	69.4869	44.2264	110.7781	-41.7061
ε=24.55						**Ethanol**					
σ_{iso}	-3.407	90.934	60.0409	153.2914	95.4098	157.7593	60.0428	157.76	88.277	-3.4101	98.2461
σ_{aniso}	166.0928	116.095	190.4559	160.5019	113.4249	104.1553	190.4549	104.1559	66.3945	166.0943	47.2147
$\Delta\sigma$	166.09275	116.09505	190.4559	160.5019	113.4249	104.15535	190.455	104.15585	66.3945	166.0944	-62.55455
η	0.933083171	0.606510355	0.736168845	0.289658163	0.329914331	0.172840377	0.736158147	0.17284251	0.879249034	0.933163309	0.50955326
δ	110.7285	77.3967	126.9706	107.0013	75.6166	69.4369	126.97	69.4372	44.263	110.7296	-41.703
ε=32.63						**Methanol**					
σ_{iso}	-3.7828	90.9093	60.1701	153.2764	95.4068	157.7673	60.1687	157.766	88.2856	-3.7834	98.2346
σ_{aniso}	166.1492	116.0777	190.3648	160.5195	113.3987	104.2414	190.3668	104.2386	66.3068	166.1465	47.1841
$\Delta\sigma$	106.9834	116.07765	190.36485	160.51945	113.3987	104.24145	190.3668	104.2386	66.30675	166.1465	-62.5581
η	0.940885085	0.607787545	0.734391091	0.289967574	0.329852696	0.17237241	0.734411147	0.172459146	0.880718026	0.938422453	0.5084905
δ	110.4662	77.3851	126.9099	107.013	75.5992	69.4943	126.9112	69.4924	44.2045	110.7644	-41.7054
ε=46.8						**DMSO**					
σ_{iso}	-3.1456	90.8955	60.2821	153.2637	95.4125	157.7789	60.2834	157.7795	88.2807	-3.15	98.2394
σ_{aniso}	166.1115	116.1375	190.2397	160.5369	113.3795	104.1508	190.2389	104.1514	66.4396	166.1145	47.2179
$\Delta\sigma$	166.11145	116.1375	190.2397	160.5369	113.37945	104.15075	190.23895	104.1514	66.4396	166.11455	-62.5547
η	0.930550563	0.605502098	0.733282082	0.28933348	0.329973818	0.174095325	0.733271568	0.174324733	0.877931378	0.930633087	0.50965036
δ	110.741	77.425	126.8265	107.0246	75.5863	69.4338	126.826	69.4343	44.2923	110.743	-41.7031
ε=2.247						**Benzene**					
σ_{iso}	-2.7375	91.1876	59.3756	153.8181	95.4262	157.5632	59.3774	157.564	88.195	-2.7392	98.3112
σ_{aniso}	165.4511	115.8775	190.5767	160.0951	113.9886	103.7904	190.5757	103.7915	66.5444	165.452	47.3772
$\Delta\sigma$	165.4511	115.8776	190.5767	160.0952	113.9886	103.7904	190.5758	103.7914	66.5444	165.452	-62.5003
η	0.921102	0.6018936	0.7491696	0.2859418	0.3290013	0.1665429	0.749158	0.1665455	0.8783195	0.9211823	0.5160595
δ	110.3007	77.2517	127.0512	106.7301	15.9924	69.1936	127.0505	69.1943	44.3629	110.3013	-41.6669

Table 3. Contd.

ε=2.023						Cyclohexane					
σ_{iso}	-2.6887	91.2063	59.3282	153.8632	95.4272	157.5459	59.3302	157.5468	88.1879	-2.693	98.3165
σ_{aniso}	165.3944	115.8586	190.5776	160.0614	114.0358	103.7618	190.5764	103.7625	66.5545	165.3965	47.3899
Δσ	165.3901	115.85865	190.5776	160.06145	114.03575	103.7618	190.5764	103.7625	66.5545	165.39645	-62.49465
η	0.920244252	0.601499758	0.750162335	0.285607317	0.328929455	0.16598602	0.750140743	0.165984821	0.878275039	0.920353187	0.51660822
δ	110.2629	77.2391	127.0517	106.7077	76.0239	69.1745	127.0509	69.175	44.3697	110.2643	-41.6631

Table 4. NMR parameters for $B_{10}N_{11}H_7(Gly)_2$ in different solvents and B3LYP/3-21G level of theory.

Atom	Gas phase										
	2N	3N	4N	7C	11N	12N	13N	20O	21O	23N	24N
σ_{iso}	189.9091	190.5401	218.2583	159.4819	145.4542	185.3316	136.2052	-67.7202	132.3026	159.9999	182.097
σ_{aniso}	78.5794	61.2344	47.615	22.1834	160.2745	73.7538	124.868	518.2375	171.968	160.2211	78.9456
Δσ	-80.8983	-77.02205	47.615	-24.71605	160.2745	-85.4029	-141.5133	518.2375	-225.9764	160.221	-91.58025
η	0.9426725	0.5900502	0.709838	0.7950587	0.519921	0.7271974	0.7647532	0.1818698	0.5220002	0.1569523	0.7240748
δ	-53.9322	-51.348	31.7433	-16.47774	106.8497	-56.9353	-94.3422	345.4916	-150.6509	106.814	-61.0535
ε=78.39						Water					
σ_{iso}	189.2264	190.1233	219.5171	159.6159	145.0224	185.323	135.0987	-64.3415	133.6487	160.8555	183.2687
σ_{aniso}	78.4289	62.1354	48.237	24.7962	159.1527	72.7294	123.7213	518.905	167.6418	158.4619	76.1951
Δσ	-80.3698	-78.28565	48.23695	-25.8231	159.1527	-84.61775	-140.7874	518.9049	-222.7409	158.4619	-88.80715
η	0.9517002	0.587405	0.549347	0.9204666	0.529107	0.7190109	0.757563	0.1850602	0.5052625	0.1546876	0.7159673
δ	-53.5799	-52.1904	32.158	-17.2154	106.1018	-56.4118	-93.8582	345.9366	-148.4939	105.6413	-59.2048
ε=32.63						Methanol					
σ_{iso}	189.2627	190.1505	219.4431	159.6156	145.043	185.3272	135.1418	-64.4821	133.5567	160.8294	183.2548
σ_{aniso}	78.447	62.097	48.1903	24.6355	159.2036	72.77	123.7708	518.8416	167.8575	158.5162	76.2696
Δσ	-80.40855	-78.23385	48.19035	-25.7386	159.2036	-84.64665	-140.8159	518.8416	-222.8877	158.5162	-88.87445
η	0.9512104	0.5874714	0.5569258	0.9142787	0.5287891	0.7193817	0.7579085	0.1843407	0.5062076	0.1547756	0.7163441
δ	-53.6057	-52.1559	32.1269	-17.1591	106.1357	-56.4311	-93.8773	345.8944	-148.5918	105.6775	-59.2496
ε=46.8						DMSO					
σ_{iso}	189.241	190.1353	219.4852	159.6164	145.0319	185.3252	135.119	-64.4026	133.6023	160.8438	183.2641
σ_{aniso}	78.4382	62.1177	48.2189	24.7253	159.1782	72.7481	123.7456	518.8698	167.7473	158.4871	76.2279
Δσ	-80.38675	-78.2631	48.21885	-25.7876	159.1782	-84.6314	-140.8014	-71.25585	-222.8108	158.4871	-88.837
η	0.95152	0.5874071	0.5525775	0.9176172	0.5289411	0.7191768	0.7577332	0.5551384	0.5057372	0.1547274	0.7161303
δ	-53.5912	-52.1754	32.1459	-17.1917	106.1188	-56.4209	-93.8676	-486.9206	-148.5406	105.6581	-59.2247

Table 4. Contd.

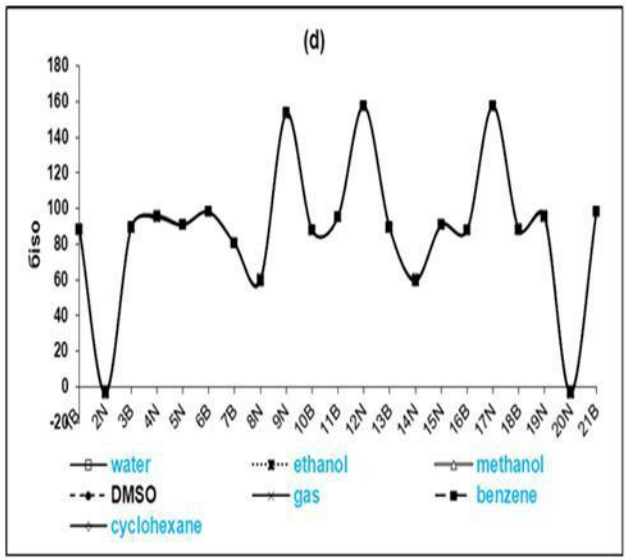
ε=2.247						**Benzene**					
σ_{iso}	189.7009	190.436	218.644	159.5565	145.307	185.3518	135.8087	-66.4568	132.5767	160.3135	182.5081
σ_{aniso}	78.5919	61.5496	47.8049	22.8665	159.9159	73.384	124.445	518.1984	170.6667	159.5839	78.0628
Δσ	-80.7739	-77.4992	47.8049	-24.92035	159.9158	-85.09805	-141.2168	518.1984	-224.9038	159.5839	-90.61185
η	0.9459641	0.5883924	0.6535948	0.8351652	0.5232665	0.7246933	0.7624665	0.1799175	0.5176862	0.1558841	0.7230164
δ	-53.8494	-51.6662	31.8699	-16.6136	106.6105	-56.732	-94.1446	345.4656	-149.9358	106.3893	-60.4079
ε=2.023						**Cyclohexane**					
σ_{iso}	189.7385	190.4554	218.5745	159.5446	145.3253	185.3503	135.8614	-66.665	132.5568	160.2697	182.4156
σ_{aniso}	78.5975	61.5058	47.7633	160.0614	159.959	73.4361	124.4945	518.2041	170.8122	159.6806	78.2358
Δσ	-80.80255	-77.4312	47.7633	-24.8613	159.959	-85.13405	-141.2491	518.2042	-225.0475	159.6806	-90.7942
η	0.9454224	0.5886542	0.6631263	0.8291924	0.522931	0.7251868	0.7627649	0.1801042	0.5180099	0.1559392	0.7233675
δ	-53.8683	-51.6208	31.8422	-16.5742	106.6393	-56.756	-94.1661	345.4695	-150.0317	106.4537	-60.5294

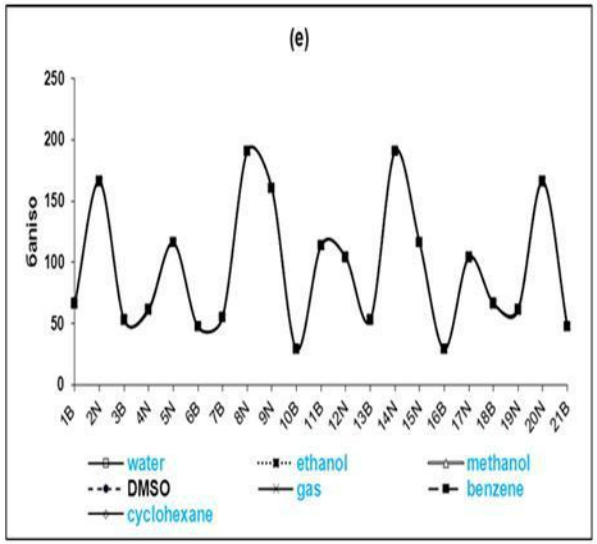
Table 5. NMR parameters for $B_{10}N_{11}H_7$ (Gly) $_2$ in different solvents and B3LYP/3-21G level of theory.

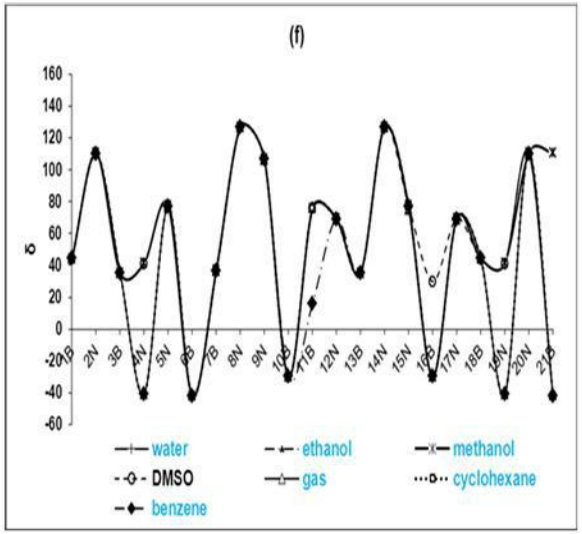
Atom	**Gas phase**										
	25N	**28B**	**29B**	**30B**	**32N**	**33N**	**34N**	**38N**	**39C**	**44O**	**45O**
σ_{iso}	137.2264	97.6816	91.0258	97.011	144.7617	191.4992	192.9215	218.1487	160.0157	-83.6915	135.8109
σ_{aniso}	124.0462	31.8346	37.2662	28.2281	157.9067	71.283	66.7787	45.122	21.4543	552.6307	189.089
Δσ	-141.4111	31.83465	37.26615	-37.8955	157.9067	-73.41055	-81.11445	45.122	-24.62335	552.6307	-215.4293
η	0.7544052	0.1938312	0.9507328	0.4897857	0.6139548	0.9420396	0.6465291	0.811082	0.7425924	0.2008973	0.7554629
δ	-94.274	21.2231	24.8441	-25.2637	105.2711	-48.9403	-54.0763	30.0813	-16.4156	368.4205	-143.6195
ε=78.39						**Water**					
σ_{iso}	137.1583	97.8019	91.1734	97.2708	145.5833	191.2243	194.2422	214.3287	159.8566	-89.7507	129.1769
σ_{aniso}	123.0016	31.9351	37.3322	28.8413	153.9994	66.9826	64.1897	47.3441	25.7865	579.3003	199.8028
Δσ	-141.2382	31.93505	37.3322	-37.7977	153.9994	-74.4509	-77.4873	47.3442	25.78645	579.3003	-231.3799
η	0.7417618	0.2145186	0.9397021	0.526089	0.6105314	0.7993754	0.6567825	0.9895003	0.9337386	0.1926881	0.7270548
δ	-94.1588	21.29	24.8881	-25.1984	102.6663	-49.634	-51.6582	31.5628	17.191	386.002	-154.253
ε=32.63						**Methanol**					
σ_{iso}	137.171	97.8053	91.1676	97.2646	145.5756	191.2362	194.2107	214.4219	159.8715	-89.6428	129.1649
σ_{aniso}	123.0377	31.9281	37.3287	28.8233	154.1166	67.0889	64.2393	47.3434	25.6739	578.7691	199.824
Δσ	-141.2524	31.9282	37.3287	-37.79975	154.1166	-74.42505	-77.5644	47.34335	25.6739	578.7691	-231.2638
η	0.7420969	0.2147941	0.9401185	0.5250558	0.6103515	0.8028567	0.656412	0.9831032	0.9398746	0.192584	0.7281041
δ	-94.1683	21.2855	24.8858	-25.1998	102.7444	-49.6167	-51.7096	31.5622	17.1159	385.8461	-154.1759

Table 5. Contd.

ε=46.8						**DMSO**					
σ_{iso}	137.1652	97.8041	91.1707	97.2682	145.581	191.2289	194.2294	214.3644	159.8626	-89.7	129.1656
σ_{aniso}	123.0195	31.932	37.3305	28.833	154.053	67.0234	64.2114	47.347	25.7416	579.0796	199.8178
Δσ	-141.2449	31.93205	31.93205	37.33045	8.4744	-74.4383	-77.51855	47.34705	25.7416	579.0796	-231.3398
η	0.7419313	0.2146702	0.2146702	0.9399003	0.9839281	0.8007778	0.656671	0.9870868	0.9363969	0.1926386	0.7274833
δ	-94.1633	21.288	21.288	24.887	56.496	-49.6255	-51.679	31.5647	17.1611	386.053	-154.2265
ε=2.247						**Benzene**					
σ_{iso}	137.2088	97.7121	91.0795	97.0997	145.0659	191.4203	193.2816	217.413	160.1542	-85.2511	132.4728
σ_{aniso}	123.6333	31.8749	37.2762	28.4504	156.638	70.5884	65.8134	45.8056	22.4388	560.0656	194.6571
Δσ	-141.3708	31.8749	37.27615	-37.8761	156.638	-73.8454	-79.97115	45.8055	-24.1514	560.0656	-221.5401
η	0.7490642	0.2026457	0.9472572	0.502291	0.6127672	0.9117899	0.6459286	0.8423748	0.8581756	0.1931897	0.7573074
δ	-94.2472	21.2499	24.8508	-25.2507	104.4253	-49.2302	-53.3141	30.537	-16.1009	373.3771	-147.6934
ε=2.023						**Cyclohexane**					
σ_{iso}	137.1964	97.6952	91.0767	97.0861	144.9957	191.4277	193.2043	217.6308	160.1403	-84.792	133.1273
σ_{aniso}	123.6746	31.8756	37.2737	28.4113	156.8535	70.8431	65.9983	45.6116	22.1842	558.065	193.5722
Δσ	-141.3578	31.87565	37.27365	-37.88253	156.8534	-73.7676	-80.21365	45.61155	-24.1843	558.065	-220.1456
η	0.7498103	0.20048	0.9477084	0.4999782	0.6133185	0.9207091	0.6455612	0.8339171	0.8345893	0.1943193	0.7585834
δ	-94.2385	21.2505	24.8491	-25.2549	104.569	-49.1784	-53.4758	30.4077	-16.1229	372.0434	-146.7637







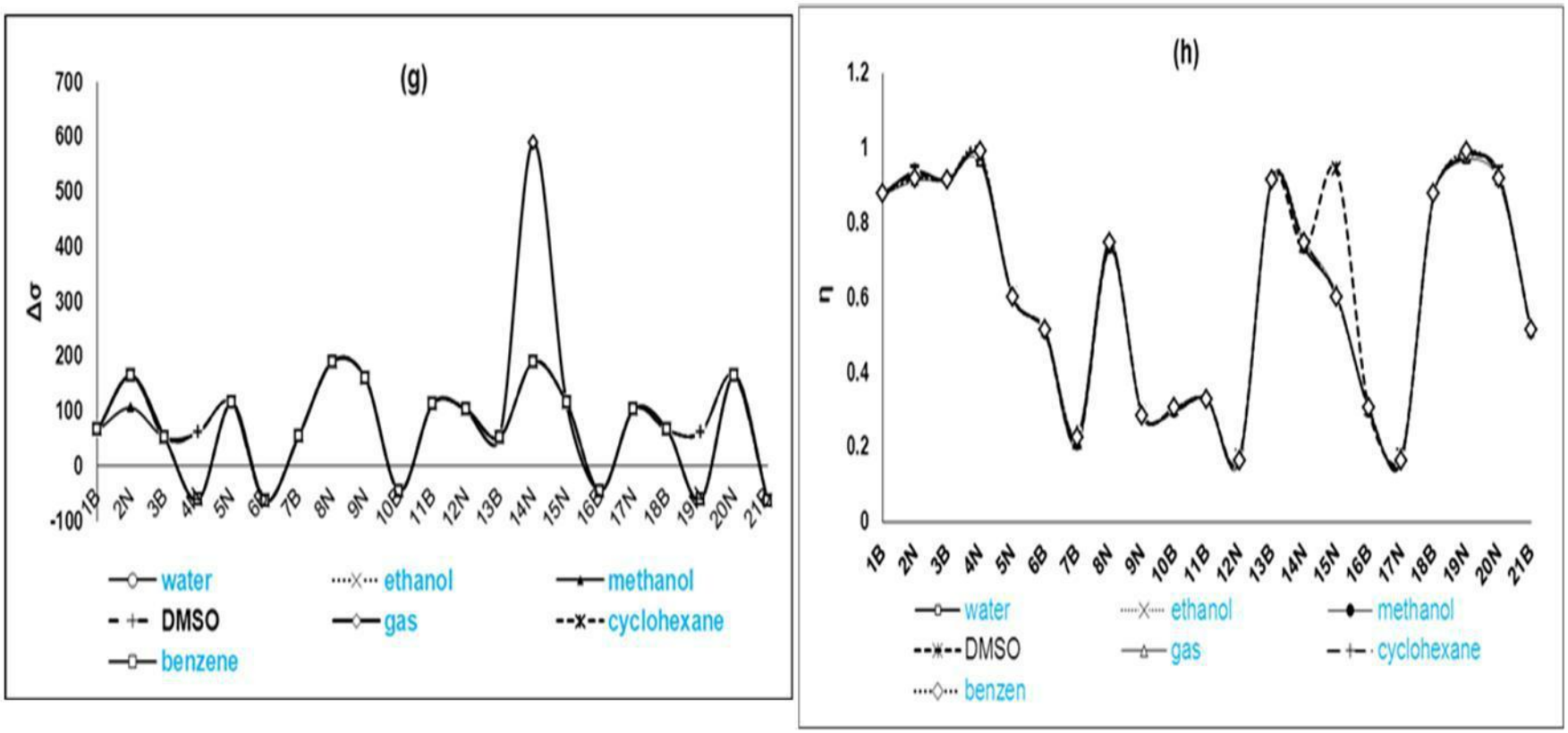


Figure 4. NMR parameters calculated: Comparison between (d) isotropy shielding (e) anisotropy shielding (f) chemical shift (g) anisotropy of the tensor and (h) asymmetry parameter for $B_{10}N_{11}$ in different solvents and B3LYP/3-21G level of theory.

applied a structure of substitutional atoms in carbon structures with disclination, called nano-cones. Then we investigated solvent effects and different temperature effects on the stability of a nanocone as $B_{10}N_{11}$ and $B_{10}N_{11}H_7$ $(Gly)_2$. For this case the values of Gibbs free energy for $B_{10}N_{11}$ nanocone were compared to each other in different solvents and temperatures which indicated the most negative value of Gibbs free energy was obtained in gas phase and 320K in B3LYP/3-21G level of theory and the same review about $B_{10}N_{11}H_7$ $(Gly)_2$ showed that the water could be suggested as the most proper solvent among different solvents which was used in this study. The results showed when temperature increases, enthalpy and energy moves toward positive values but Gibbs free energy moves toward nega-tive values. Finally our major results from the point of view of solvent effects can be summarized that gas phase is the best phase for $B_{10}N_{11}$ nanocone and water solvent is the best medium for $B_{10}N_{11}H_7$ $(Gly)_2$ so the greater stability for $B_{10}N_{11}$ was obtained in Gas phase and for $B_{10}N_{11}H_7$ $(Gly)_2$ was computed in water solvent and these results for these structures were obtained in 320 K.

As it is known the value of dipole moment depends on dielectric constant solvent and increase of dielectric constant solvent increases the dipole moment.

Then Mulliken charges and NMR parameters

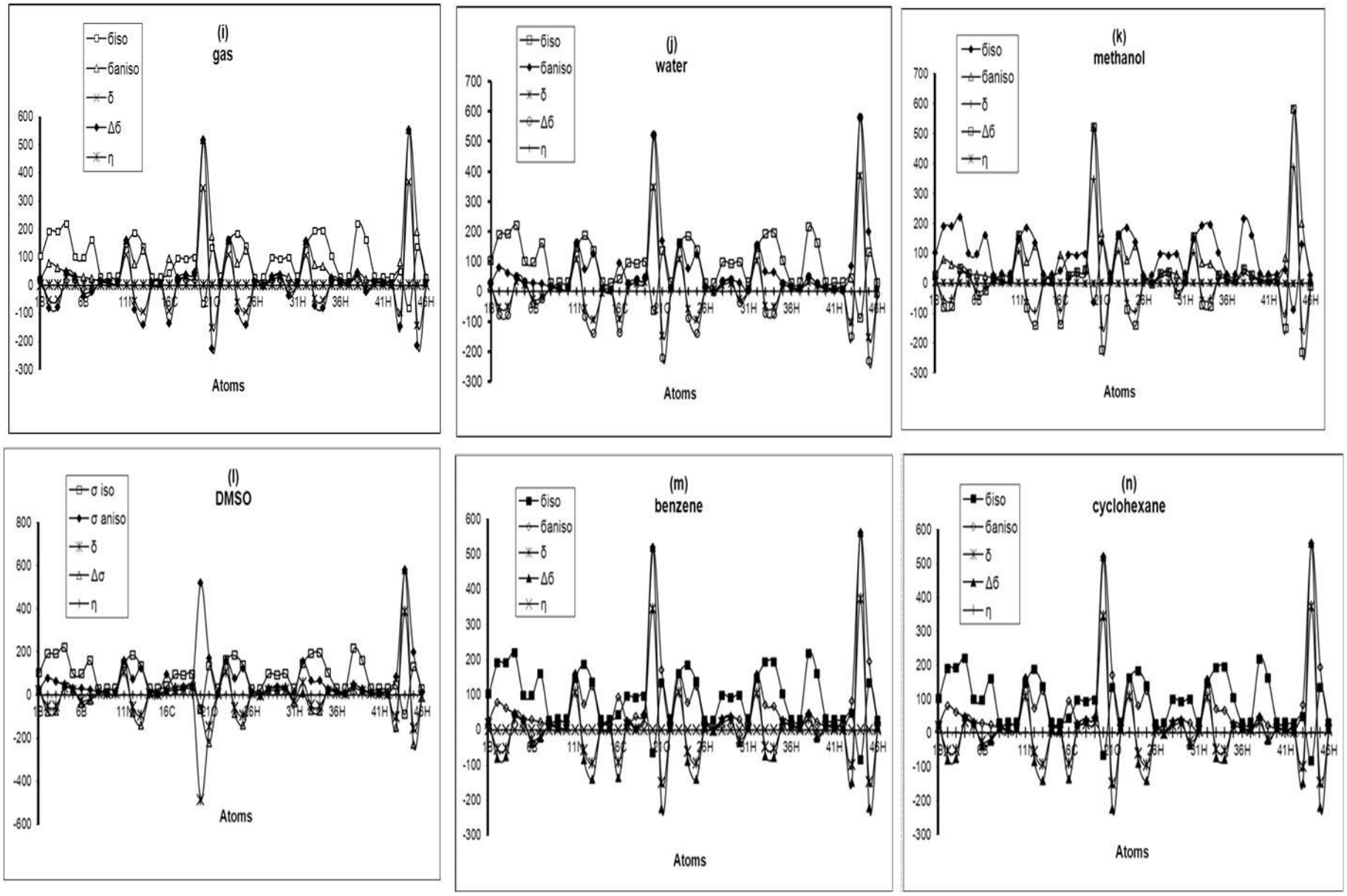


Figure 5. Calculated of NMR parameters for $B_{10}N_{11}H_7$ (Gly) $_2$ in different solvents :(i) gas phase (j) w ater (k) methanol (l) DMSO (m) benzene (n) cyclohexane in B3LY P/3-21G level of theory.

Table 6. The values of Mulliken charges for per atom of $B_{10}N_{11}$ nanocone in different solvents and B3LYP/3-21G level of theory.

Atoms	Solvents						
	Gas	Water	Ethanol	Methanol	DMSO	Benzene	Cyclohexane
1B	0.471699	0.454702	0.455598	0.45524	0.455045	0.464791	0.46559
2N	-0.5446	-0.5462	-0.54608	-0.54611	-0.54623	-0.54513	-0.54506
3B	0.788056	0.778102	0.778698	0.778362	0.778422	0.78406	0.78452
4N	-0.52682	-0.52902	-0.52892	-0.52891	-0.52906	-0.52767	-0.52756
5N	-0.73631	-0.73732	-0.73738	-0.73723	-0.73739	-0.73681	-0.73675
6B	0.675926	0.682487	0.68206	0.682289	0.682294	0.678417	0.678111
7B	0.749136	0.760194	0.759572	0.759794	0.760086	0.753505	0.752981
8N	-0.49844	-0.50147	-0.50129	-0.50135	-0.50144	-0.49958	-0.49944
9N	-0.78161	-0.78144	-0.78149	-0.78143	-0.78146	-0.78157	-0.78157
10B	0.741894	0.756342	0.755708	0.755797	0.756198	0.747832	0.747145
11B	0.733423	0.751111	0.750089	0.75051	0.750811	0.740401	0.739573
12N	-0.72189	-0.72256	-0.72249	-0.72253	-0.72257	-0.72208	-0.72205
13B	0.788056	0.778101	0.778698	0.778361	0.778422	0.784059	0.784519
14N	-0.49844	-0.50147	-0.50129	-0.50135	-0.50145	-0.49958	-0.49944
15N	-0.73631	-0.73732	-0.73738	-0.73723	-0.73739	-0.73681	-0.73675
16B	0.741895	0.756343	0.755708	0.755798	0.756198	0.747833	0.747146
17N	-0.7219	-0.72256	-0.72249	-0.72253	-0.72257	-0.72208	-0.72205
18B	0.471695	0.454698	0.455594	0.455236	0.455042	0.464786	0.465585
19N	-0.52682	-0.52902	-0.52892	-0.52891	-0.52905	-0.52767	-0.52756
20N	-0.5446	-0.5462	-0.54608	-0.54611	-0.54623	-0.54513	-0.54505
21B	0.675931	0.68249	0.682065	0.682292	0.682298	0.678423	0.678117

Table 7. The values of Mulliken charges for per atom of $B_{10}N_{11}H_7(Gly)_2$ in different solvents and B3LYP/3-21G level of theory.

Atoms	Solvents					
	Gas	Water	Methanol	DMSO	Benzene	Cyclohexane
1B	0.917265	0.915562	0.91571	0.915622	0.917125	0.917232
2N	-0.85013	-0.84809	-0.84818	-0.84814	-0.84948	-0.84954
3N	-0.8193	-0.8175	-0.81758	-0.81754	-0.81874	-0.81883
4N	-0.72503	-0.72524	-0.72522	-0.72524	-0.72508	-0.72507
5B	0.804042	0.801177	0.801326	0.801246	0.803364	0.803497
6B	0.796388	0.781324	0.781896	0.781595	0.790838	0.791543
7C	-0.29976	-0.3063	-0.30608	-0.30619	-0.30225	-0.30193
8H	0.307556	0.312207	0.311975	0.312106	0.309015	0.308782
9H	0.264517	0.277108	0.276673	0.276894	0.269428	0.268845
10H	0.28727	0.298836	0.298425	0.298632	0.291694	0.291173
11H	-0.81467	-0.81315	-0.81321	-0.81318	-0.8141	-0.81416
12N	-0.81012	-0.81005	-0.81006	-0.81005	-0.81017	-0.81017
13N	-0.79625	-0.79554	-0.79557	-0.79555	-0.79604	-0.79607
14H	0.227859	0.25306	0.25211	0.252602	0.237208	0.236031
15H	0.228705	0.234794	0.234504	0.234663	0.230629	0.230334
16C	0.644519	0.650825	0.650568	0.650709	0.64679	0.646465
17B	0.848165	0.839021	0.839424	0.839218	0.84511	0.845512
18B	0.785336	0.764935	0.765706	0.765309	0.777854	0.7788
19B	0.489701	0.475424	0.475937	0.475675	0.48425	0.484912
20O	-0.47266	-0.48558	-0.48511	-0.48535	-0.47753	-0.47695
21O	-0.54349	-0.53105	-0.53154	-0.53128	-0.53897	-0.53956
22H	0.266847	0.276181	0.275876	0.276031	0.270626	0.270186

Table 7. Contd.

23N	-0.82553	-0.82367	-0.82374	-0.8237	-0.82486	-0.82495
24N	-0.80786	-0.80894	-0.80893	-0.80893	-0.80825	-0.80817
25N	-0.79607	-0.79611	-0.79612	-0.79611	-0.7961	-0.79608
26H	0.368541	0.370542	0.370342	0.370448	0.36857	0.368519
27H	-0.04157	-0.04248	-0.04249	-0.04248	-0.0423	-0.04224
28B	0.806153	0.799346	0.799683	0.799511	0.80374	0.803987
29B	0.786571	0.75967	0.7607	0.760168	0.776838	0.778088
30B	0.780679	0.761324	0.762069	0.761687	0.773148	0.77399
31H	0.269259	0.276853	0.276604	0.276729	0.272457	0.272105
32N	-0.81179	-0.81203	-0.81204	-0.81204	-0.8119	-0.81184
33N	-0.85484	-0.8534	-0.85353	-0.85346	-0.85472	-0.8547
34N	-0.81619	-0.81655	-0.8166	-0.81658	-0.81604	-0.81594
35B	0.919801	0.938498	0.938123	0.938363	0.924131	0.922916
36H	0.294058	0.290581	0.290517	0.290536	0.293532	0.293995
37H	0.282833	0.283906	0.283831	0.283872	0.282888	0.282846
38N	-0.72317	-0.72798	-0.72787	-0.72793	-0.72442	-0.72412
39C	-0.29714	-0.30135	-0.30124	-0.30129	-0.29948	-0.29923
40H	0.289979	0.290659	0.290596	0.290629	0.290054	0.290009
41H	0.229815	0.247307	0.246769	0.247047	0.236835	0.235887
42H	0.223181	0.238988	0.238404	0.238707	0.228843	0.228076
43C	0.626286	0.620387	0.62051	0.620428	0.625412	0.625821
44O	-0.46434	-0.46875	-0.46833	-0.46856	-0.46415	-0.46418
45O	-0.54549	-0.54061	-0.54079	-0.5407	-0.54395	-0.54424
46H	0.370064	0.365851	0.365918	0.365879	0.368112	0.368412

Table 8. Calculated Dipole moments (Debye) of $B_{10}N_{11}$ nanocone and $B_{10}N_{11}H_7$ $(Gly)_2$ versus dielectric constant at B3LYP/3-21G level of theory.

Structure	μ (Debye)	Gas	Water	Methanol	DMSO	Benzene	Cyclohexane
		ε=1	ε=78.39	ε=32.63	ε=46.8	ε=2.247	ε=2.023
B10N11		4.3860	5.6347	5.5945	5.6098	4.8848	4.8262
B10N11H7(Gly)2		9.3875	13.4930	13.3510	13.4254	10.8911	10.6785

were employed to determine the location of active sites. A good agreement was observed between Mulliken charges and NMR parameters. On the other hand, to show the location of active sites, NMR parameters and Mulliken charges can be used. The results show, $B_{10}N_{11}$ nanocone is a good detector of biological molecules such as amino acids. Finally, our results confirm the role of $B_{10}N_{11}$ nanocone as a better candidate in biological systems and drug delivery than the other nanostructures.

REFERENCES

Becke AD (1992). Density functional thermochemistry. II. The effect of the Perdew–Wang generalized gradient correlation. J. Chem. Phys., 97: 9173.

Becke AD (1992). Density functional thermochemistry. I. The effect of the exchange only gradient correction. J. Chem. Phys., 96: 2155-2160.

Becke AD (1993). Density-functional thermochemistry. III. The role of exact exchange. J. Chem. Phys., 98: 5648-5652.

Bethune DS (1993). Cobalt-catalysed growth of carbon nanotubes with single-atomic-layer walls. Nature (London), 363: 605-606.

Bourgeois L, Bando Y, Han WQ, Sato T (2000). Structure of boron nitride nanoscale cones: Ordered stacking of 240 degrees and 300 degrees disclinations. Phys. Rev. B., 61: 7686-7691.

Charlier JC, Rignanese GM (2001). Electronic structure of carbon nanocones. Phys. Rev. Lett., 86: 5970-5973.

De Dios AC, Roach JL, Walling AE (1999). The NMR Chemical Shift: Local Geometry Effects. ACS Symposium Series, 732: 220-239.

Iijima S (1991). Helical microtubules of graphitic carbon. Nature (London), 354: 56-58.

Iijima S, Ichihashi T (1993). Single-shell carbon nanotubes of 1-nm diameter. Nature (London), 363: 603-604.

Iijima S, Ichihashi T, Ando Y (1992). Pentagons, Heptagons and Negative Curvature in Graphite Microtubule Growth. Nature, 356: 776-778.

Kroto HW, Health JR, O'Brien SC, Curl RF, Smalley RE (1985). C60: Buckminsterfullerene. Nature (London), 318: 162-163.

Machado M, Mota R, Piquini P (2003). Electronic properties of BN nanocones under electric fields. Microelectronics J., 34: 545-547.

Mollaamin F, Baei MT, Monajjemi M, Zhiani R, Honarparvar B (2008). A DFT study of hydrogen chemisorption on v (100) surfaces. Russian J. Phys. Chem. A., 82: 2354-2361.

Mollaamin F, Gharibe S, Monajjemi M (2011). Synthesis of various nano and micro ZnSe morphologies by using hydrothermal method. Inter. J. Phys. Sci., 6: 1496-1500.

Monajjemi M, Baei MT, Mollaamin F (2008). Quantum mechanic study of hydrogen chemisorptions on nanocluster vanadium surface. Russian J. Inorganic Chem., 53: 1430-1437.

Monajjemi M, Heshmat M, Tahan A, Monajemi H, Mollaamin F (2007). Quantum mechanic study of basis set effect on NMR chemical shielding and Hydrogen bonding of some amino acids in gaseous phase and solvent. Egypt. J. Biochem. Mol. Biol., (BIANNUAL), 25: 154-179.

Monajjemi M, Lee VS, Khaleghian M, Honarparvar B, Mollaamin F (2010). Theoretical Description of Electromagnetic Nonbonded Interactions of Radical, Cationic, and Anionic NH2BHNBHNH2 Inside of the B18N18 Nanoring. J. Phys. Chem., 114: 15315-15330.

Monajjemi M, Mahdavian L, Mollaamin F (2008). Characterization of nanocrystalline silicon germanium film and nanotube in adsoption gas by monte carlo and langevin dynamic simulation. Bull. Chem. Soc. Ethiop., 22: 277-286.

Monajjemi M, Rajaeian E, Mollaamin F, Naderi F, Saki S (2008). Investigation of NMR shielding tensors in 1,3 dipolar cycloadditions: solvents dielectric effect. Phys. Chem. Liquids., 46: 299-306.

Monajjemi M, Razavian MH, Mollaamin F, Naderi F, Honarparvar B (2008). A Theoretical thermochemical study of solute-solvent dielectric effects in the displacement of codon-anticodon base pairs. Russian J. Phys. Chem. A., 82: 2277-2285.

Nirmala V, Kolandaivel P (2007). Structure and electronic properties of armchair boron nitride nanotubes. J. Mol. Structure, Theochem., 817: 137-145.

Oku T, Nishiw aki A ,Narita I, Gonda M (2003). Formation and structure of B24N24 clusters. Chem. Phys. Lett., 380: 620-623.

Rubio A, Corkill JL, Cohen ML (1994). Theory of graphitic boron nitride nanotubes. Phys. Rev. B., 49: 5081-5084.

Sachdeva H, Müllera FB, Hüfnerb S (2010). BN analogues of graphene: On the formation mechanism of boronitrene layers — solids with extreme structural anisotropy. Diamond Related Mater., 19: 1027-1033.

Terauchi M, Tanaka M, Suzuki M, Ogino A, Kimura K (2000). Production of zigzag-type BN nanotubes and BN cones by thermal annealing. Chem. Phys. Lett ., 324: 359-364.