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*Full Length Research Paper*

# NMR Shielding and thermodynamic density functional theory (DFT) studies of solvent effect on $B_{10}N_{11}H_7(Ala)_2$ Nano Cone

**M. Monajjemi[1]*, N. Hooshmand[2], H. Seyed Hosseini Ghaheh[3] and F. Mollaamin[4]**

[1]Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran.
[2]Science and Research Branch, Islamic Azad University, Tehran, Iran.
[3]Young Researchers Club, Science and Research Branch, Islamic Azad University, Tehran, Iran.
[4]Department of Chemistry, Qom Branch, Islamic Azad University, Qom, Iran.

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**B3LYP/3-21G density functional theory (DFT) are carried out on the structure and stability of $B_{10}N_{11}H_7(Ala)_2$ in bulk and different solvent medium, using Gaussian 98 package of program. NMR parameters and thermodynamic properties were calculated to obtain stability and solvent effect. It was found that computationally efficient solvent modeling is possible to find better results and also molecular structure of $B_{10}N_{11}H_7(Ala)_2$. The results show that, because of high stability of $B_{10}N_{11}$ nanocone, it can be the best candidate and much favorable in biological systems and drug delivery.**

**Key words:** Solvent effect, density functional theory (DFT), NMR parameters, $B_{10}N_{11}H_7(Ala)_2$, nanocone, thermodynamic properties.

## INTRODUCTION

Most studies have been conducted on carbon nanotubes (Iijima, 1991; Iijima and Ichihashi, 1993; Bethune et al., 1993) and C60 (Kroto et al., 1985), since they have been discovered. Many novel structures such as carbon nanocones, and boron nitride nanocones have been viewed as intermediate between nanotubes and grapheme sheet (Sattler, 1995; Zhi et al., 2005). Because of their unique properties than those of carbon structure, more recently nanocones are more focused by scientist Iijima et al. (1992) 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 (Rubio et al., 1994), with employing various theoretical and experimental techniques to investigate properties of nanocones (Qu et al., 2008; Zhang et al., 2007), but most of these studies have been performed experimentally (Bourgeois et al., 2000).

The fascinating novel structures of boron nitride (BN) (Rubio et al., 1994) have been intensively studied, since they have unique and interesting properties such as electronic (Song et al., 1994; Yakobson and Smalley, 1997) and mechanical properties (Depres et al., 1995; Iijima et al., 1996).

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 better candidates to predict properties compare to other composite materials. BNNCs have been investigated and synthesized (Bourgeois et al., 2000; Rubio et al., 1994), and they have very interesting properties when compared with similar carbon nanostructure (Terauchi et al., 2000).

We have proposed a $B_{10}N_{13}$ nanocone as a particular case to attach to alanine, trough B terminated atoms to investigate thermodynamic properties. BN nanocones are widely applicable in many fields such as cold electron source (Baylor et al., 2002; Dean and Chamala, 1999), and probes for electronic microscopy devices. The purpose of this work is to understand stability, atomic structure and thermochemistry properties of one of the particular Boron Nitride nanocones as $B_{10}N_{11}H_7(Ala)_2$.The

*Corresponding author. m_monajjemi@yahoo.com.

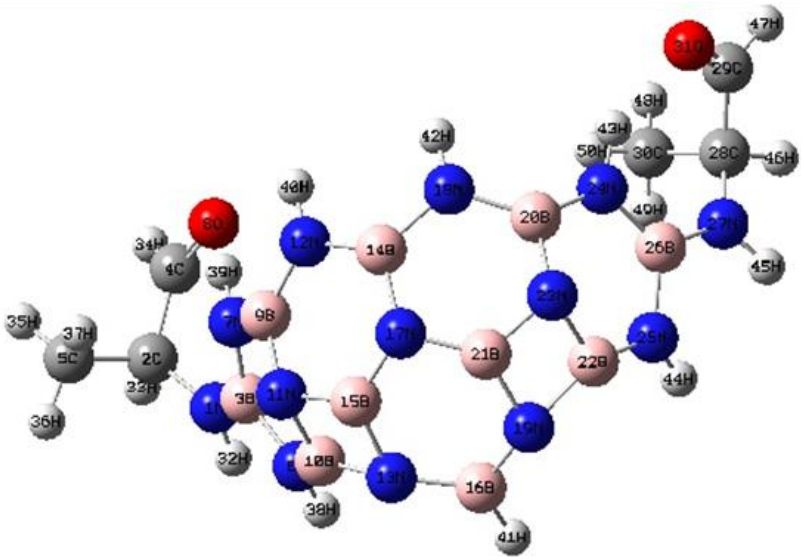



**Figure 1.** 3D view of $B_{10}N_{11}H_7(Ala)_2$, where pink , blue, red, gray and light gray sphere indicate B , N, O, C and H atoms respectively .

BN nanocones are the structures with polarity and high reactivity and flexibility to reagent medium surrounded, because the negative charge at B atom positions and also positive charge at N atom positions. In this research, solvent effect has been performed, using onsager self-consistent model reaction field (SCRF) to analysis of thermodynamic parameters, and calculating Gibbs free energy, enthalpy and dipole moment. We have also computed the Mulliken charge and found active sites to obtain Nuclear magnetic resonance (NMR) parameters.

## COMPUTATIONAL DETAILS

In this study, all the calculations have been performed using of the *Gaussian 98* program in the electronic ground state (Frisch 1998). We used this package to predict many properties of our system such as molecular energies and structures, thermodynamic properties, atomic charges, multiple moment and NMR shielding in both gas phase and different solvent.

Density functional theory (DFT) (Becke, 1992a, b) is a computational method that is frequently used in computing properties of macromolecules so we applied this method to study $B_{10}N_{11}H_5(Ala)_2$. The hybrid DFT used in this research is B3LYP [21-25] /3-21Glevel of theory for geometry optimizations. Frequency test at the optimized structures has been done at the same theoretical level to clarify the optimized structure and wave function is ground state, without imaginary frequencies. Solvent effect was calculated in different solvents and temperatures by using the same method and basis sets. We have also computed average charge to obtain active sites in B10N11H7 $(Ala)_2$.

NMR spectroscopy is extremely sensitive to molecular structure and also environmental effects (Evans, 1995; Kaupp et al., 2004; Otting and Liepinsh, 1995; Monajjemi et al., 2007; 2008). To obtain deeper physical insight into the influence of the solvent effect we also calculated NMR parameters for two cases (1) solute in the gas phase and (2) solute in the different solvent mediums. In all calculations the default gaugae-including atomic orbital (GIAO) [33] orbitals were used to obtain molecular magnetic susceptibilities, NMR shielding with Gaussian program.

## RESULTS AND DISCUSSION

$B_{10}N_{13}$ nanocone as a particular case was considered to attach to Alanine, trough B terminated atoms. The resulting BN nonocones were simulated by (BN) Ala containing 10 B atoms plus 15 N atoms, to investigate stability as well as thermodynamic properties. The results have given in Tables 1-4 and five Figures 1-5 as follows. The optimization structure has been carried out to find ground state structure shown in Figure 1. The computed energetic data (the electronic energy, the electronic energy with zero-point energy correction $E_0$, zero point energy ZPE, enthalpy H, E and Gibbs free energy G) as well as dipole moment for various solvent are given in Table 1 and Table 2 respectively. To make our analysis clear and easier, $B_{10}N_{11}H_7$ $(Ala)_2$ is divided in six layers of atoms (or active sites) as shown in Figure 3. These six layers constituted by: (1) five atoms; (2) two atoms; (3) three atoms; (4) three atoms; (5) one atom ; (6) one atom. We choose these particular layers due to the location of more negative (N atoms) and positive electronic charge (B atoms). The calculated Mulliken charge values per atom per layer are shown in Figure 4 and Table 3. The NMR parameters were computed with concentration on active sites, shown in Figure 5 and data summarized in Table 4.

## Conclusion

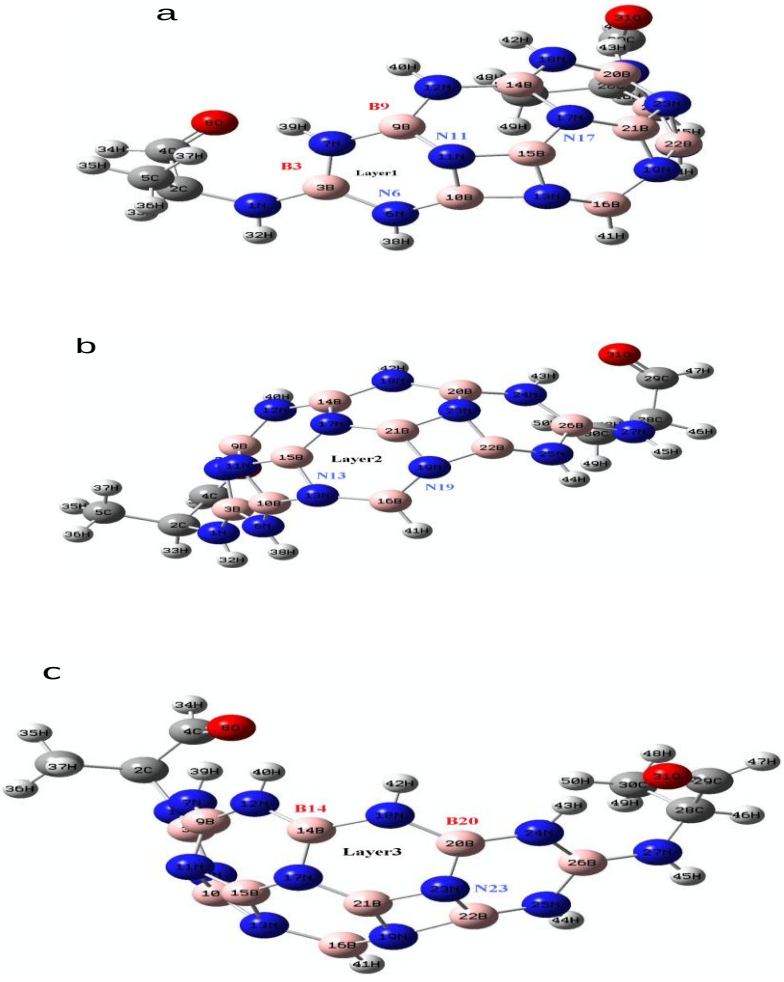
In summary, theoretical calculation at the level of B3LYP/3-21G level on $B_{10}N_{11}H_7(Ala)_2$ nanocone have been performed. All calculations indicated that $B_{10}N_{11}$

**Table 1.** Relative energy E and $E_0$ (with ZPE correction a.u.) Free energies G (a.u.) and Enthalpies H (a.u.), ZPE (a.u.) for $B_{10}N_{11}H_7(Ala)_2$ at B3LYP/3-21G level of theory.

| Solvent | E | $E_0$ | H | G | ZPE |
|---|---|---|---|---|---|
| water | -1344.009897 | -1344.036623 | -1344.008953 | -1344.094042 | 0.376856 |
| DMSO | -1344.010962 | -1344.036819 | -1344.010017 | -1344.092215 | 0.376782 |
| ethanol | -1344.010065 | -1344.036815 | -1344.009121 | -1344.094536 | 0.376834 |
| methanol | -1344.010008 | -1344.036751 | -1344.009064 | -1344.094355 | 0.376841 |
| benzene | -1344.014448 | -1344.041059 | -1344.013504 | -1344.097458 | 0.377064 |
| gas phase | -344.014449 | -44.041060 | -344.013505 | -1344.097458 | 0.377064 |

**Table 2.** calculated dipole moment μ (Debye) versus dielectric constant for $B_{10}N_{11}H_7(Ala)_2$ at B3LYP/3-21G in five different solvents and gas phase.

| Medium | Dielectric constant (ε) | μ (Debye) |
|---|---|---|
| water | 78.39 | 12.1588 |
| DMSO | 46.8 | 12.0911 |
| ethanol | 24.55 | 12.0635 |
| methanol | 32.63 | 12.0966 |
| benzene | 2.247 | 9.0180 |
| gas phase | 1 | 9.0193 |



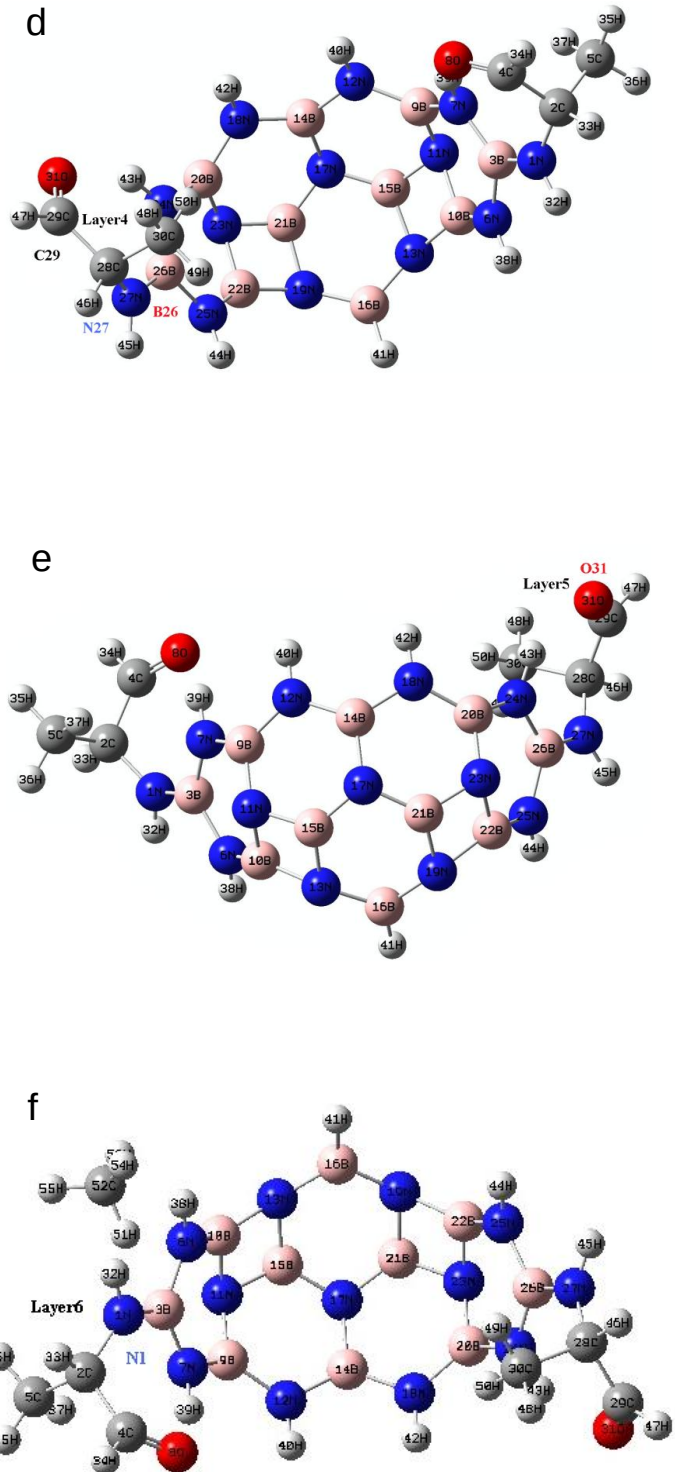



**Figure 2.** (a) 3D view of the layer1, (b) 3D view of the layer 2, (c) 3D view of the layer 3, (d) 3D view of the layer 4, (e) 3D view of the layer 5, (f) 3D view of the layer 6.

$H_7(Ala)_2$ nancone structure possesses lower energy. The computed energy of the studied structure shown and proved the high stability of system without distortion and also more stable in different solvents. As a general result, it was found that the medium is basically not affected by different dielectric constant on stability. Further, to determine the location of active sites, Mulliken charge and NMR parameters were also analyzed. This is

**Table 3.** Average Mulliken charge values per atom per layer for $B_{10}N_{11}H_7(Ala)_2$ in five different solvents and gas phase.

| | | Charge on atoms | | | | | |
|---|---|---|---|---|---|---|---|
| **Layer** | **Atoms** | **gas** | **DMSO** | **water** | **Methanol** | **Ethanol** | **Benzene** |
| Layer 1 | B3 | 0.924636 | 0.924482 | 0.924478 | 0.924537 | 0.924565 | 0.925129 |
| | B9 | 0.800731 | 0.790008 | 0.789848 | 0.790203 | 0.790394 | 0.798106 |
| | N11 | -0.81334 | -0.81046 | -0.81038 | -0.810499 | -0.810559 | -0.812603 |
| | N6 | -0.54113 | -0.53187 | -0.53164 | -0.532038 | -0.532256 | -0.53771 |
| | N17 | -0.82592 | -0.82334 | -0.8233 | -0.823363 | -0.823401 | -0.825402 |
| Layer 2 | N13 | -0.79727 | -0.79546 | -0.79541 | -0.795475 | -0.795512 | -0.796835 |
| | N19 | -0.79702 | -0.79458 | -0.79452 | -0.794576 | -0.794608 | -0.79664 |
| Layer 3 | B20 | 0.81421 | 0.794121 | 0.793719 | 0.794306 | 0.794622 | 0.809787 |
| | N23 | -0.81454 | -0.80925 | -0.80917 | -0.809232 | -0.809267 | -0.814249 |
| | B14 | 0.849512 | 0.831462 | 0.831106 | 0.831674 | 0.831979 | 0.845374 |
| Layer 4 | B26 | 0.949052 | 0.91256 | 0.91182 | 0.912198 | 0.912389 | 0.949109 |
| | N27 | -0.45566 | -0.45125 | -0.4516 | -0.451616 | -0.451625 | -0.454291 |
| | C29 | 0.457787 | 0.479295 | 0.479726 | 0.479181 | 0.478894 | 0.453605 |
| Layer 5 | O31 | -0.4261 | -0.41356 | -0.41424 | -0.413693 | -0.413412 | -0.426326 |
| Layer 6 | N1 | -0.45383 | -0.44667 | -0.44641 | -0.446745 | -0.446937 | -0.451212 |

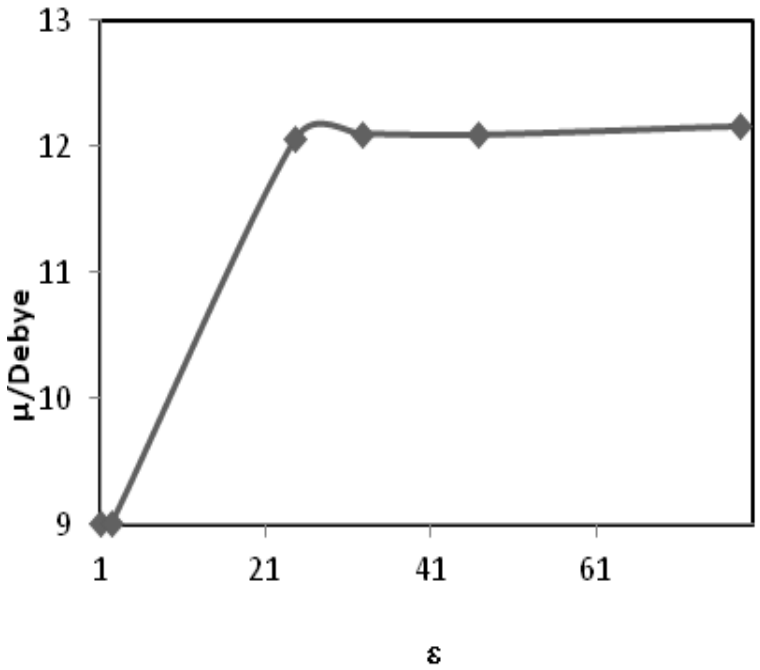



**Figure 3.** Calculated dipole moment μ (Debye) versus dielectric constant at bulk and five different solvents.

important to fully understand the geometrical specialty of $B_{10}N_{11}H_5$ $(Ala)_2$ nanocone and the few other recently reported faceted nanocones, more favorable energetically and stability and could be the best candidate in biological system and drug delivery instead of the other nanocompounds.

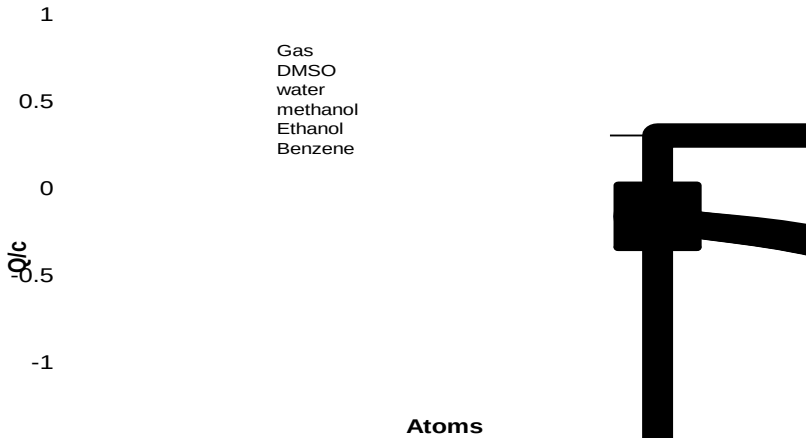
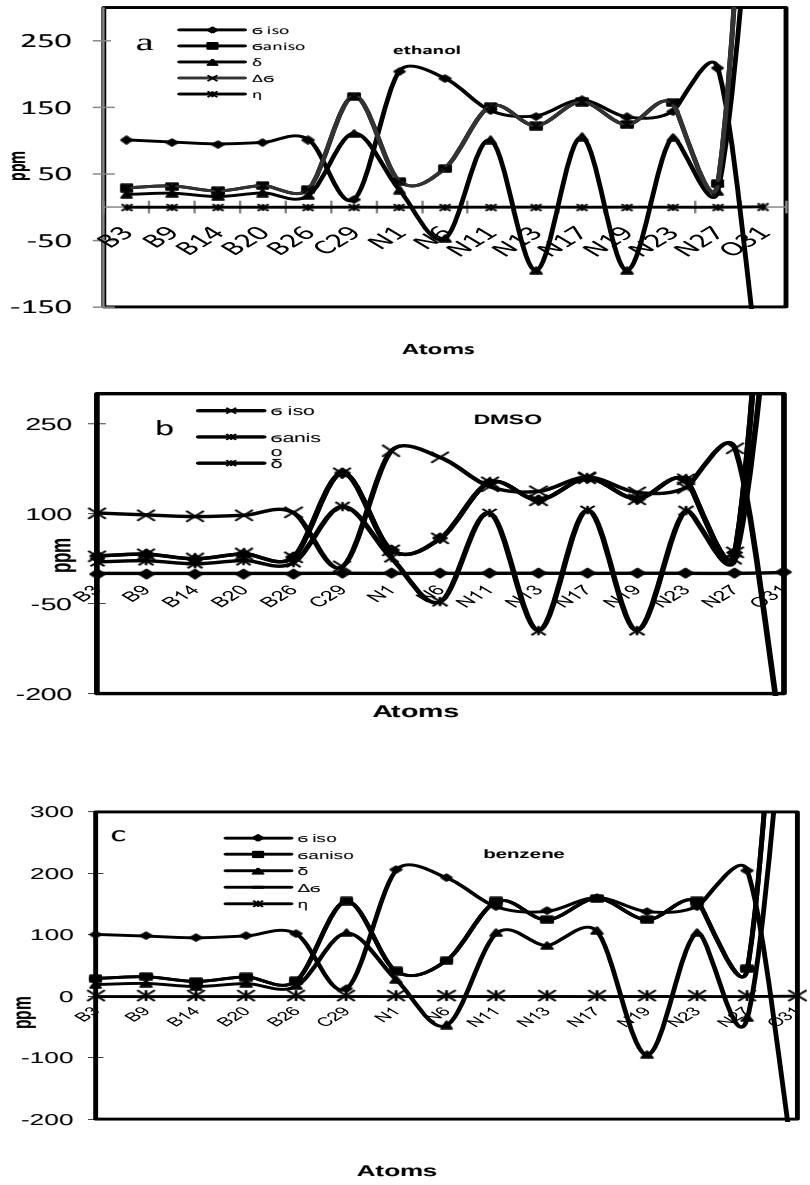



**Figure 4.** Average Mulliken charge values per atom for $B_{10}N_{11}H_7(Ala)_2$ in five different solvents and gas phase.



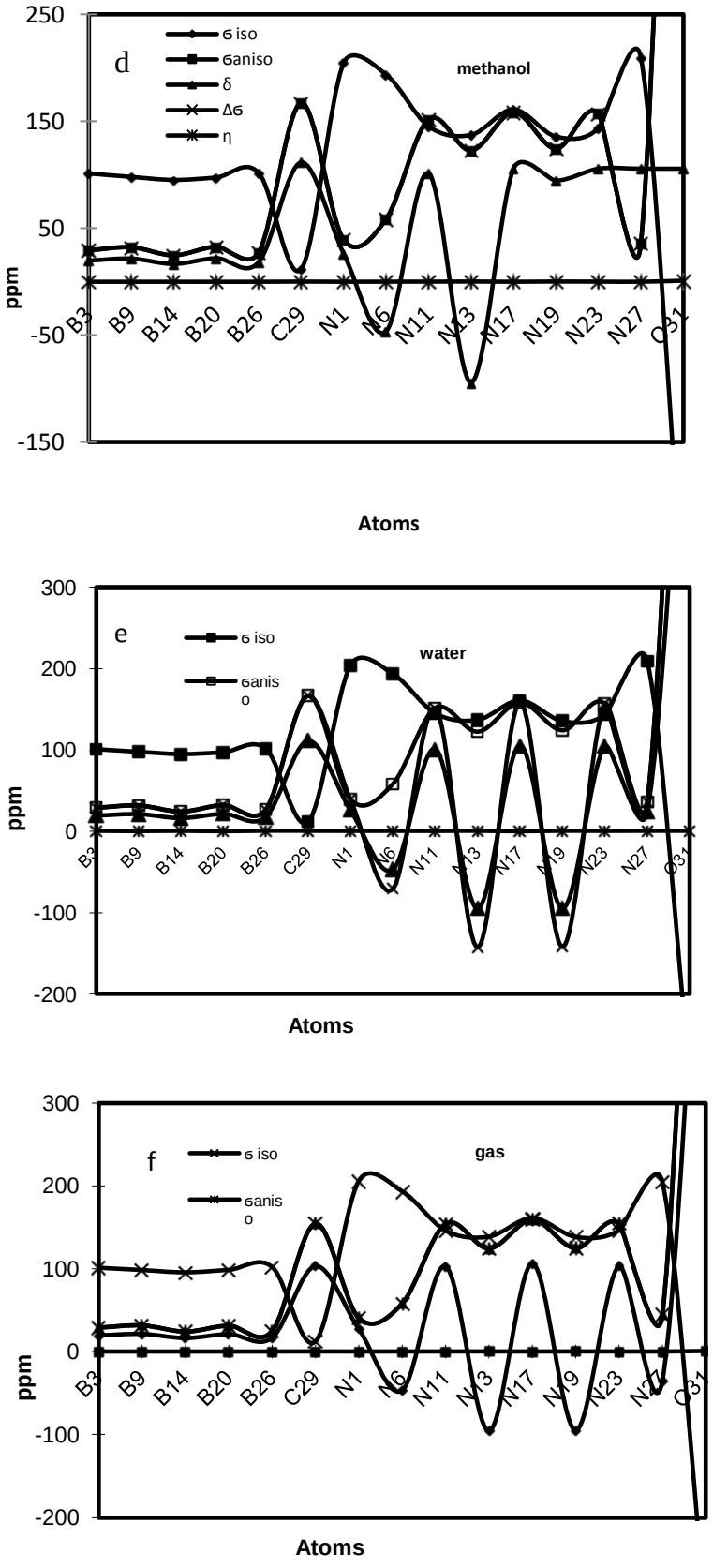



**Figure 5.** NMR parameters calculated (B3LYP/32-G) for $B_{10}N_{11}H_7(Ala)_2$ in (a) ethanol, (b) DMSO, (c) benzene, (d) methanol, (e) water and (f) gas Phase.

**Table 4.** computed NMR parameters for $B_{10}N_{11}H_7(Ala)_2$ in five different solvents and gas phase.

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | **Gas phase** | | | | | | | | |
| **Atoms** | **B3** | **B9** | **B14** | **B20** | **B26** | **C29** | **N1** | **N6** | **N11** | **N13** | **N17** | **N19** | **N23** | **N27** | **O31** |
| **σiso** | 100.9465 | 98.2129 | 95.4131 | 98.4160 | 101.8399 | 12.28930 | 205.7754 | 192.9488 | 145.6830 | 138.4417 | 160.8857 | 138.1028 | 146.1919 | 204.5292 | -313.47300 |
| **σaniso** | 29.07860 | 31.7621 | 24.3325 | 31.4200 | 25.01910 | 154.5290 | 40.52490 | 58.24060 | 154.1514 | 124.4176 | 159.0033 | 124.6511 | 154.7576 | 44.44420 | 1046.7968 |
| **δ** | 19.38580 | 21.1748 | 16.2217 | 20.9467 | 16.67940 | 103.0194 | 27.01660 | -46.89490 | 102.7676 | -95.8712 | 106.0023 | -95.0613 | 103.1717 | -35.3264 | 697.86450 |
| **Δσ** | 29.10000 | 31.8000 | 24.3000 | 31.4000 | 25.10000 | 155.0000 | 40.50000 | 5.820000 | 154.0000 | 124.000 | 159.0000 | 125.000 | 155.0000 | 44.4000 | 1050.0000 |
| **η** | 0.019900 | 0.01220 | 0.01770 | 0.00646 | 0.020900 | 0.109000 | 0.027800 | 0.078800 | 0.080300 | 0.15600 | 0.024800 | 0.15300 | 0.084900 | 0.05880 | 0.7340000 |
| **[** | | | | | | | | **Water** | | | | | | | |
| **σiso** | 101.0527 | 97.8058 | 95.0031 | 97.2640 | 101.5386 | 11.77650 | 204.395 | 193.5692 | 145.1282 | 137.0782 | 161.0010 | 135.4905 | 143.2476 | 209.2982 | -297.2700 |
| **σaniso** | 29.17440 | 32.0125 | 24.5057 | 32.5700 | 27.06550 | 166.9395 | 39.0502 | 58.54650 | 151.7222 | 122.6105 | 158.3841 | 124.3154 | 157.0553 | 35.93250 | 998.2299 |
| **δ** | 19.44960 | 21.3417 | 16.3371 | 21.7134 | 18.04360 | 111.2930 | 26.0335 | -46.83090 | 101.1481 | -94.71570 | 105.5894 | -94.50270 | 104.7035 | 23.95500 | 665.4866 |
| **Δσ** | 29.17440 | 32.0125 | 24.5057 | 32.5700 | 27.06540 | 166.9395 | 39.0502 | -70.24630 | 151.7223 | -142.0740 | 158.3841 | -141.7540 | 157.0553 | 35.93250 | 998.2299 |
| **η** | 0.696700 | 0.37880 | 0.70820 | 0.21130 | 0.807600 | 0.731500 | 0.61940 | 0.666900 | 0.561300 | 0.726000 | 0.163300 | 0.754000 | 0.618700 | 0.726900 | 0.716200 |
| **[** | | | | | | | | **DMSO** | | | | | | | |
| **σiso** | 101.0485 | 97.8135 | 95.0084 | 97.2699 | 101.5543 | 11.41390 | 204.5011 | 193.5591 | 145.1567 | 137.1130 | 160.9926 | 135.5404 | 143.2728 | 208.9999 | -299.22100 |
| **σaniso** | 29.17170 | 32.0102 | 24.5089 | 32.5788 | 27.07540 | 167.7433 | 39.10780 | 58.51930 | 151.7326 | 122.6498 | 158.4052 | 124.3351 | 157.0788 | 35.70260 | 1001.2873 |
| **δ** | 19.44780 | 21.3401 | 16.3393 | 21.7192 | 18.05030 | 111.8289 | 26.07190 | -46.82530 | 101.1551 | -94.74540 | 105.6035 | -94.52550 | 104.7192 | 23.80170 | 667.52480 |
| **Δσ** | 0.029200 | 0.03200 | 0.02450 | 0.03260 | 0.027100 | 0.167700 | 0.039100 | -70.23800 | 0.151700 | -142.1180 | 0.158400 | -141.7880 | 0.157100 | 0.035700 | 1.0013000 |
| **η** | 0.696800 | 0.37890 | 0.70910 | 0.21300 | 0.806500 | 0.720400 | 0.620400 | 0.000100 | 0.561100 | 0.726000 | 0.163300 | 0.753800 | 0.618300 | 0.714400 | 0.7172000 |
| **[** | | | | | | | | **Ethanol** | | | | | | | |
| **σiso** | 101.0471 | 97.82800 | 95.0156 | 97.2810 | 101.550 | 11.61500 | 204.5035 | 193.5597 | 145.1829 | 137.1646 | 160.9687 | 135.5665 | 143.2798 | 209.1777 | -298.0310 |
| **σaniso** | 29.17320 | 32.00270 | 24.5115 | 32.5603 | 27.0577 | 167.2675 | 39.10630 | 58.50600 | 151.8033 | 122.7014 | 158.4600 | 124.3879 | 157.1806 | 35.88060 | 999.4545 |
| **δ** | 19.44920 | 21.33520 | 16.3409 | 21.7069 | 18.0385 | 111.5117 | 26.07090 | -46.8085 | 101.2022 | -94.76780 | 105.6399 | -94.53960 | 104.7871 | 23.92040 | 666.3030 |
| **Δσ** | 29.20000 | 32.00000 | 24.5000 | 32.6000 | 27.1000 | 167.0000 | 39.10000 | 58.5000 | 152.0000 | 123.0000 | 158.0000 | 124.0000 | 157.0000 | 35.90000 | 999.0000 |
| **η** | 0.020300 | 0.012100 | 0.01740 | 0.00694 | 0.02190 | 0.122000 | 0.024300 | 0.08200 | 0.085200 | 0.162000 | 0.025900 | 0.159000 | 0.097200 | 0.026000 | 0.717000 |
| **[** | **Methanol** | | | | | | | | | | | | | | |
| **σiso** | 101.0491 | 97.8200 | 95.0114 | 97.2746 | 101.5466 | 11.66610 | 204.4602 | 193.5638 | 145.1634 | 137.1336 | 160.9803 | 135.5403 | 143.2672 | 209.2151 | -297.7980 |
| **σaniso** | 29.17380 | 32.0059 | 24.5093 | 32.5643 | 27.06000 | 167.1669 | 39.08400 | 58.52120 | 151.7740 | 122.6710 | 158.4335 | 124.3616 | 157.1343 | 35.89140 | 999.0795 |
| **δ** | 19.44920 | 21.3372 | 16.3395 | 21.7096 | 18.04000 | 111.4446 | 26.05600 | -46.8169 | 101.1827 | -94.75070 | 105.6223 | 94.52610 | 105.6223 | 105.6223 | 105.6223 |
| **Δσ** | 29.20000 | 32.0000 | 24.5000 | 32.6000 | 27.10000 | 167.0000 | 39.10000 | 58.5000 | 152.0000 | 123.0000 | 158.0000 | 124.0000 | 157.0000 | 35.90000 | 999.0000 |
| **η** | 0.020300 | 0.01210 | 0.0174 | 0.00693 | 0.021900 | 0.122000 | 0.024300 | 0.08200 | 0.085200 | 0.162000 | 0.025900 | 0.159000 | 0.097300 | 0.026100 | 0.717000 |

**Table 4.** Continues.

| [ | | | | | | | | Benzene | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **σiso** | 100.9459 | 98.2135 | 95.4118 | 98.4161 | 101.8400 | 12.28280 | 205.7742 | 192.949 | 145.6834 | 138.4446 | 160.8832 | 138.1041 | 146.1893 | 204.5426 | -313.5010 |
| **σaniso** | 29.07910 | 31.7617 | 24.3337 | 31.4174 | 25.01940 | 154.5376 | 40.52330 | 58.2409 | 154.1528 | 124.4169 | 159.0048 | 124.6568 | 154.7742 | 44.45060 | 1046.854 |
| **δ** | 19.38600 | 21.1745 | 16.2225 | 20.9449 | 16.67960 | 103.0250 | 27.01550 | -46.8931 | 102.7686 | 82.94460 | 106.0032 | -95.06290 | 103.1827 | -35.3209 | 697.9027 |
| **Δσ** | 29.10000 | 31.8000 | 24.3000 | 31.4000 | 25.00000 | 155.0000 | 40.50000 | 58.2000 | 145.0000 | 124.0000 | 159.0000 | 125.0000 | 155.0000 | 44.5000 | 1050.000 |
| **H** | 0.019900 | 0.01220 | 0.01770 | 0.00645 | 0.020900 | 0.109000 | 0.027800 | 0.07870 | 0.080300 | 0.156000 | 0.02480 | 0.153000 | 0.084900 | 0.05880 | 0.734000 |

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