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Full Length Research Paper

Monte Carlo and density functional theory (DFT) investigation of boron-nitride nano cones in different solvents

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Quantum Monte Carlo (QMC), molecular dynamics (MD) simulations and density functional theory (DFT) calculations at the level of B3LYP/3-21G was carried out on the structure and stability of $B_{10}N_{11}H_7$ $(Thr)_2$ in bulk and different solvent medium. NMR parameters and thermodynamic properties were calculated to obtain chemical shift, stability and solvent effect. It was found that computationally efficient solvent modeling is possible and can reveal fine details of molecular structure, stability and dynamics. The results showed 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: Molecular dynamics, density functional theory (DFT), $B_{10}N_{11}H_7(Thr)_2$, nanocone, Monte Carlo.

INTRODUCTION

Most of the studies have been done 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 nano-cones and boron nitride nanocones have been viewed as intermediate between nanotubes and graphene sheet (Sattler, 1995; Zhi et al., 2005).

As a result of their unique properties than those of carbon structure, in recent years there has been a great interest in studying the properties of the nanocones 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 theore-tical and experimental research. Studies and the publi-cations on nanocones have been on since 1994 (Rubio et al., 1994) with employing various theoretical and experi-mental techniques to investigate valuable properties of nanocones (Rubio et al., 1994; Qu et al., 2008) 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 (Depres et al., 1995; Iijima et al., 1996) properties. Boron Nitride 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 (Rubio et al., 1994; Bourgeois et al., 2000; Terauchi et al., 2000) and shown they have very interesting properties in comparison with similar carbon nanostructure. We have proposed a $B_{10}N_{13}$ nanocone as a particular case to attach to Threonin, trough B terminated atoms to investigate thermodynamic properties. BNNCs are widely applicable in many fields such as cold electron source (Baylor et al., 2002; Monajjemi et al., 2010), 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 BNNCs as $B_{10}N_{11}H_7$ $(Thr)_2$.

The BN nanocones are the structures with polarity and

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high reactivity and flexibility to reagent medium surrounded, because the negative charge at N atom positions and also positive charge at B atom positions. In present work based on DFT calculations, molecular dynamic simulation (MD) (Atkins and Friedman, 1997; Billing and Mikkelsen, 1997) and quantum Monte Carlo (QMC) (Monajjem et al., 2006; Monajjemi et al., 2006), we have simulated $B_{10}N_{11}H_7$ $(Thr)_2$ structure and investigated its properties. In this research, solvent effect has been performed, using onsager self-consistent model reaction field (SCRF) for the 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 NMR parameters.

COMPUTATIONAL DETAILS

In present work, all calculations were performed using the *Gaussian98* program (Frisch et al., 1998) in the electronic ground state. We used this package to study many specific properties of $B_{10}N_{11}H_7$ $(Thr)_2$ such as molecular energies and structures, thermodynamic properties, Atomic charges, Multipole moment and NMR shielding in both gas phase and different solvent.

Density functional theory (DFT) (Parr and Yang, 1989) is a general computational method that is frequently used in computing properties of macromolecules as we applied this method to study on $B_{10}N_{11}H_7$ $(Thr)_2$. The atomic orbitals generally described by analytical basis set, and a basis set consisting of many atomic functions, gives better description of the electronic structure of the system. The Becke 3 Lee-Yang-Parr (B3LYP) functional (Becke, 1993; Parr and Yang, 1989) with 3-21G split-valance basis set was used in this work. Complete geometry optimizations for $B_{10}N_{11}H_7$ $(Thr)_2$ were carried out at B3LYP /3-21G level of theory. We have performed frequency test at the same theoretical level to clarify the optimized structure and wave function is ground state, without imaginary frequencies. MD and QMC simulations are two methods for determining physical properties of macroscopic, they were used to find additional minima in the present work. In both methods, the standard program package was used and the temperature T is sequentially increased, step by step, from room temperature (RT, 300K) to 310K.

Solvent effect on $B_{10}N_{11}H_7$ $(Thr)_2$ was calculated in different solvents and five different temperatures of 298, 300, 305, 310 and 315K by using the same method and basis sets. The average atomic charges have been derived from DFT calculations to obtain active sites in $B_{10}N_{11}H_7$ $(Thr)_2$.

It is well known that NMR spectroscopy is extremely sensitive to molecular structure and also environmental effects (Parr and Yang, 1989; Monajjemi et al., 2005, 2007, 2008; Kaupp et al., 2004; Otting and Liepinsh, 1995).

NMR investigation gives deeper physical insight into the influence of the solvent effect. In this work NMR parameters were calculated in 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) (Donald and Martin, 2009), 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 Threonin (Thr), trough B terminated atoms. The resulting BNNCs were simulated by (BN) Thr containing 10 B atoms plus 13 N atoms, to investigate stability as well as thermodynamic properties. Except for some test cases we have used B3LYP/3-21G level of theory for geometry optimization of $B_{10}N_{11}H_7$ $(Thr)_2$. The results have given in four tables and six figures as follow. Full geometry optimization of $B_{10}N_{11}H_7$ $(Thr)_2$ has been carried out to find ground state structure shown in Figure 1. Figures 2 and 3 showed dependency of dipole moment to solvent dielectric constant and NMR parameters in five different solvents and gas phase respectively. A very good agreement can be observed between the calculated average Mulliken charges and medium in Figure 4. As it shown in Figures 5 and 6, we have prepared our system for MD and QMC simulations for four different temperatures of 300, 305, 310 and 315K. In each case we followed standard default of MD and QMC simulations and performed a series of the calculations under a constant temperature and environmental setup with the interval of $0 < t < 100$ ps and $0 < t < 0.1$ ps for QMC and MD respectively. Using DFT method, the computed energetic data (enthalpy H, internal energy E and Gibbs free energy G) as well as dipole moment for various solvent are given in Table 1 and 2 respectively. To make our analysis clear and easier, $B_{10}N_{11}H_7$ $(Thr)_2$ is divided in three layers of atoms (or active sites) as shown in Table 3. These four layers constituted by: (1) six atoms, (2) three atoms, (3) five atoms, (4) seven atoms. 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 Table 3. The NMR parameters were computed with concentration on active sites, and data summarized in Table 4.

Conclusions

In summary, an analysis of the MD, QMC and DFT calculations at the level of B3LYP/3-21G on $B_{10}N_{11}H_7$ $Thr)_2$ nanocone have been performed. All calculations indicated that $B_{10}N_{11}H_7$ $(Thr)_2$ 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. Further, to determine the location of active sites, Mulliken charge and NMR parameters were also analyzed and the modeling provided chemical shift to study not only molecular structure, but also the specific solvent-solute interactions. The calculated results were strongly dependent on the adopted QMC and MD simulations. This is important to fully understand the geometrical specialty of $B_{10}N_{11}H_5$ $(Thr)_2$ nanocone and the few other recently reported faceted nanocones, more favorable energetically and stability. With regard to bio-chemical phenomena, the results, illustrate a new picture of the BNNCs as a favorable candidate in biological system,

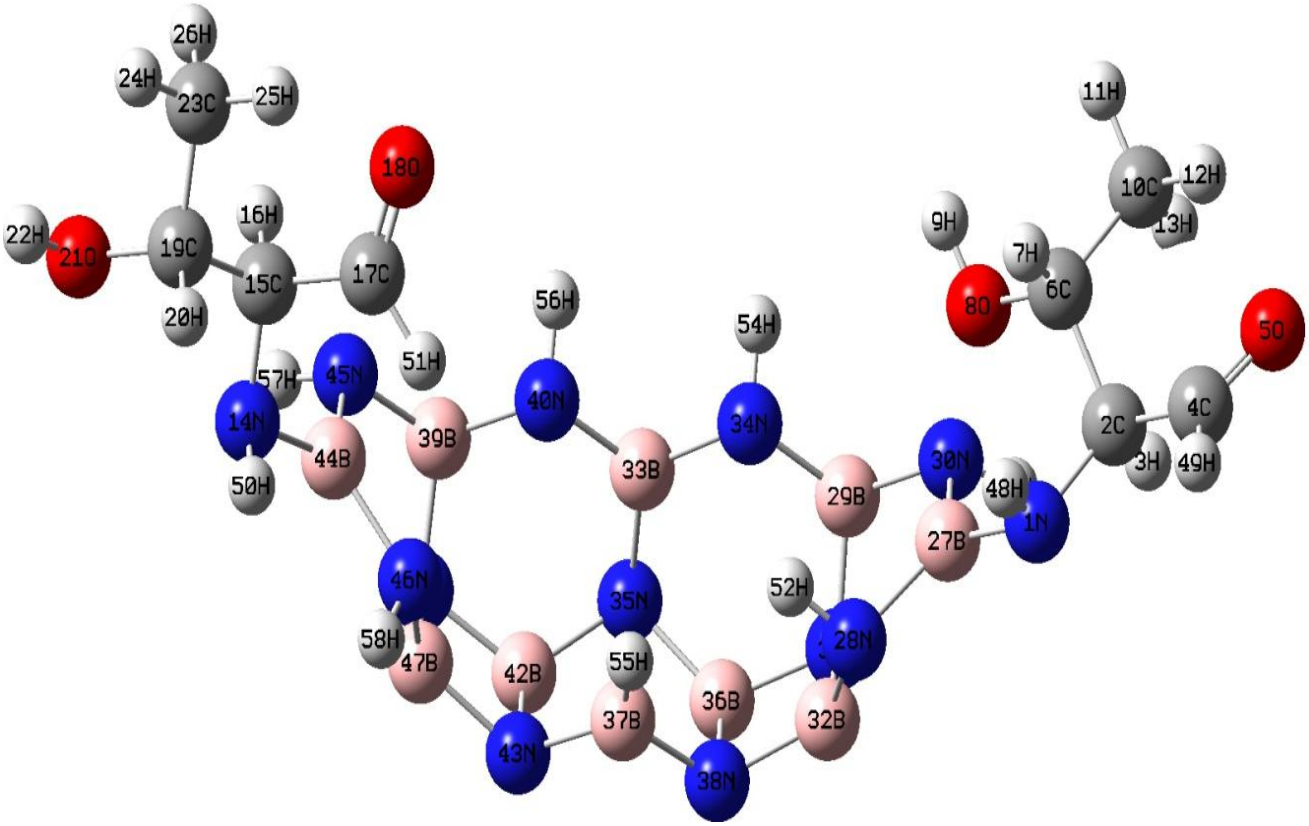

Figure 1. 3D view of $B_{10}N_{11}H_7$ $(Thr)_2$, where pink, blue, red, gray and light gray sphere indicate B, N, O, C and H atoms respectively.

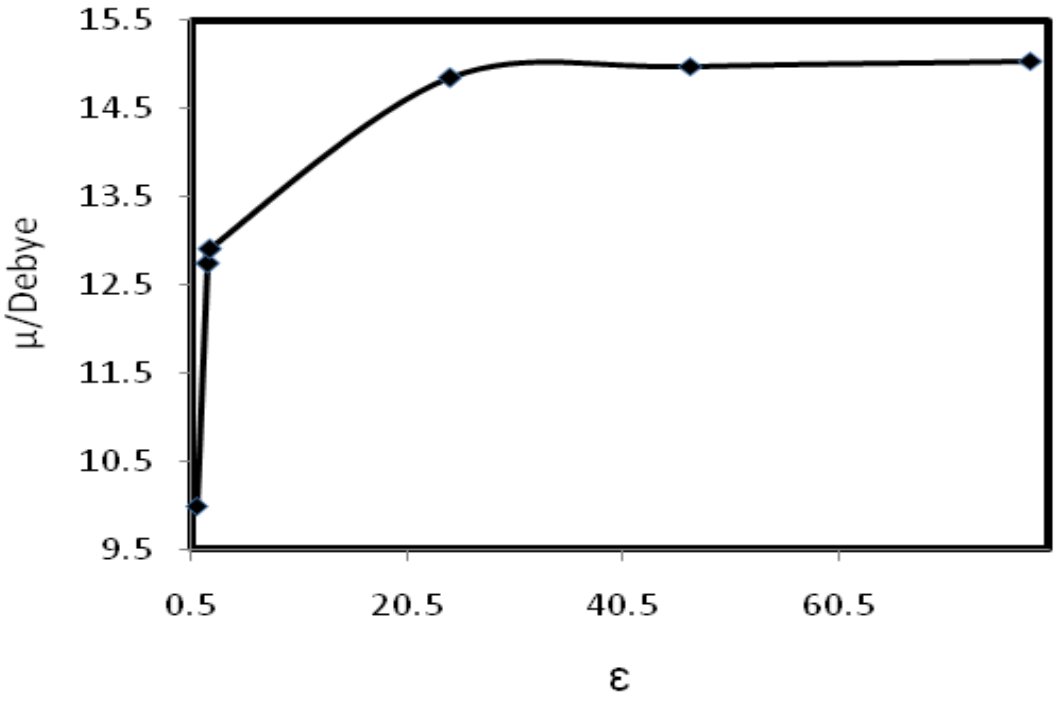

Figure 2. Calculated dipole moment μ (Debye) versus dielectric constant (ε) at bulk and five different solvents.

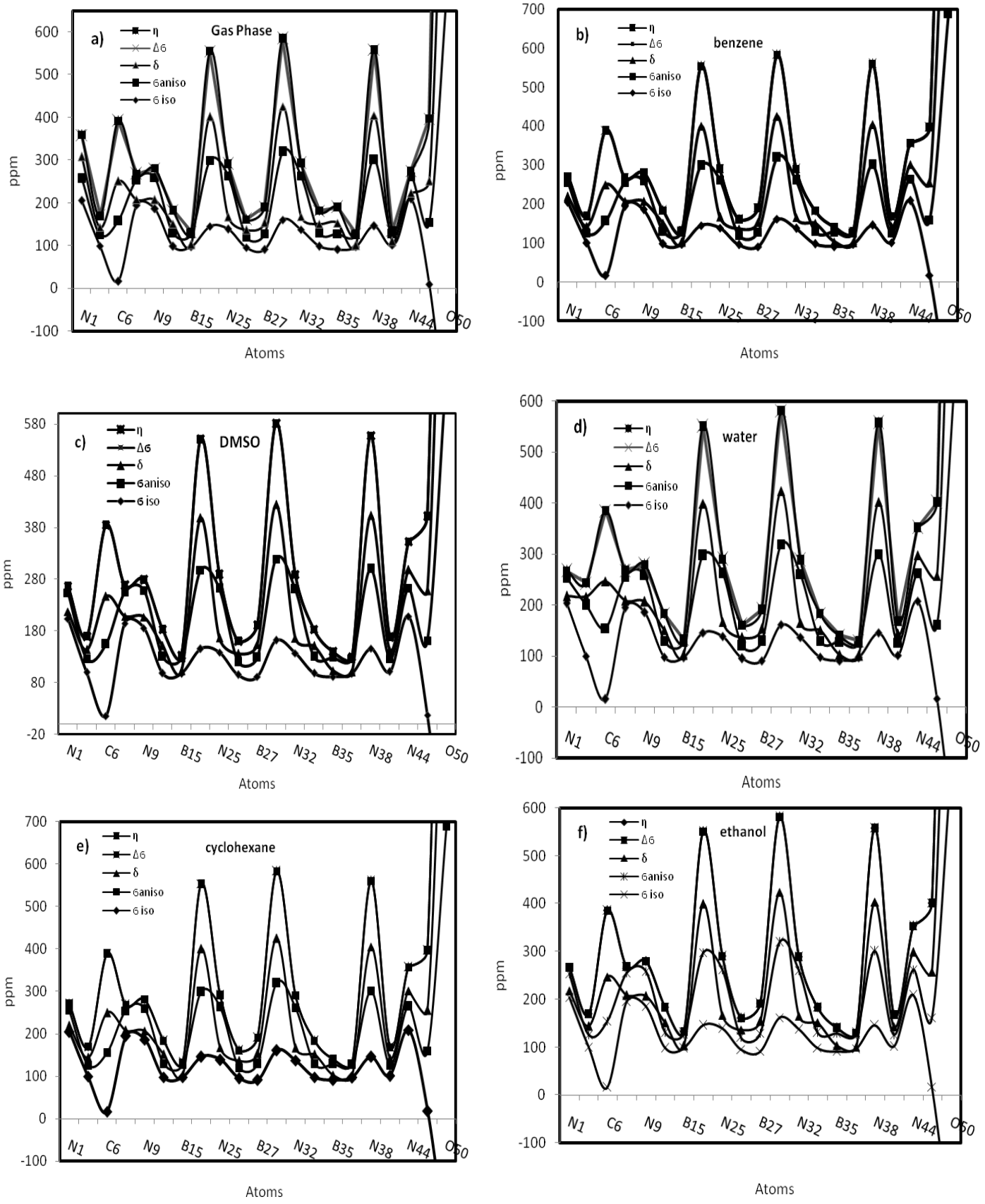

Figure 3. NMR parameters calculated (B3LYP/32-G) for $B_{10}N_{11}H_7$ $(Thr)_2$ in (a) gas phase, (b) benzene, (c)DMSO, (d) water (e) cyclohexane, (f) ethanol.

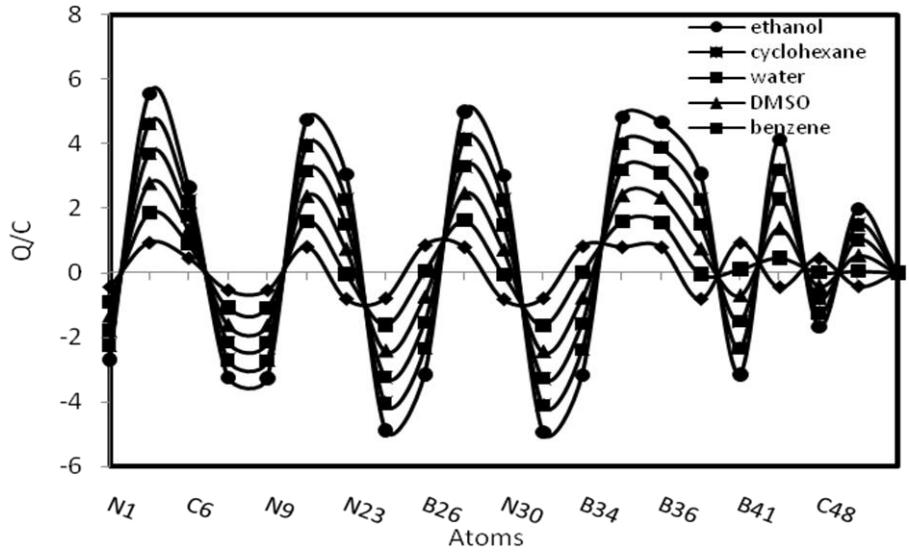

Figure 4. Average Mulliken charge values per atom for $B_{10}N_{11}H_7(Thr)_2$ in five.

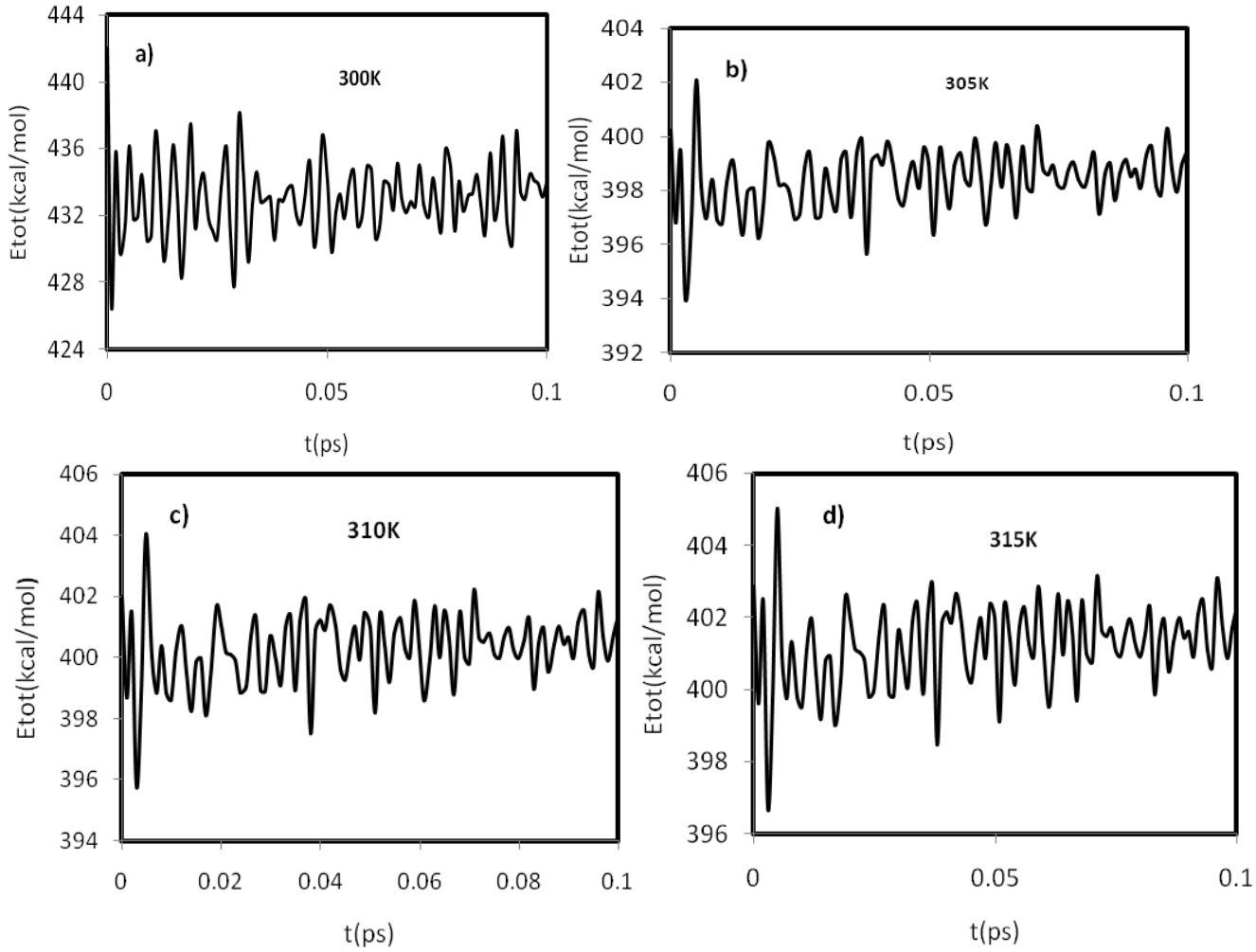

Figure 5. MD Calculations for $B_{10}N_{11}H_7(Thr)_2$: under four different temperatures and environmental setup with the interval of $0 < t < 0.1$ ps.

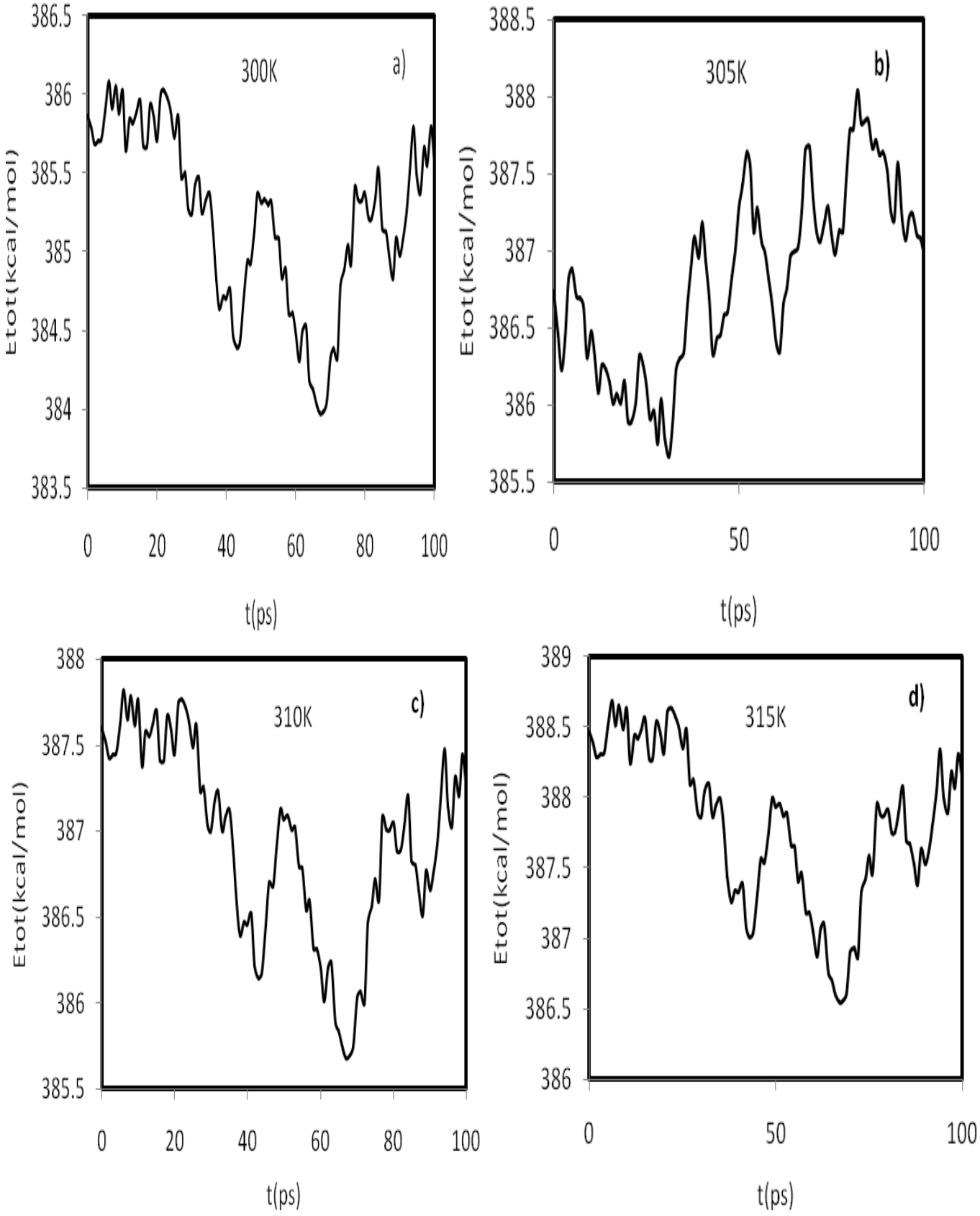

Figure 6. QMC Calculations for $B_{10}N_{11}H_7(Thr)_2$: under four different temperatures and environmental setup with the interval of $0 < t < 100$ ps.

Table 1. Computed energetic data ,enthalpy H (kcal/mol), internal energy E (kcal/mol) and Gibbs free energy G (kcal/mol) for $B_{10}N_{11}H_7(Thr)_2$.

Temperature			298 K	300 K	305 K	310 K	315 K
Phase	Gas ε=1	-G(Kcal/mol)	986338.5027	986338.87987442	986339.90773498	986340.9456356	986341.99483158
		-H(Kcal/mol)	986277.7786	986277.54333083	986276.90201612	986276.2506612	986275.59114878
		-E(Kcal/mol)	986278.371015	986278.139464862	986277.5075627	986276.8668755	986276.21677575
	Water ε=78.39	-G(Kcal/mol)	986337.6756	986338.046541808	986339.0574596	986340.0784175	986341.11004318
		-H(Kcal/mol)	986277.961252	986277.726563611	986277.0865039	986410.8207009	986275.77940163
		-E(Kcal/mol)	986278.553621	986278.323325145	986277.6926780	986277.0532459	986276.40502860
	Ethanol ε=24.55	-G(Kcal/mol)	986337.721491	986338.092977511	986339.1032678	986340.1242257	986341.15522387
		-H(Kcal/mol)	986278.016473	986277.781784447	986277.1417247	986276.4922524	986275.83399495
		-E(Kcal/mol)	986278.608841	986278.377918472	986277.7478989	986277.1084667	986276.46024944
	DMSO ε=46.8	-G(Kcal/mol)	986337.688861	986338.060347017	986339.0706373	986340.0915952	986341.12322088
		-H(Kcal/mol)	986277.979449	986277.745388896	986277.1047016	986276.4558568	986275.79759940
		-E(Kcal/mol)	986278.572446	986278.341522921	986277.7108758	986277.0714436	986276.42322637
	Benzene ε=2.247	-G(Kcal/mol)	986338.128745	986338.500231176	986339.5105214	986340.5321069	986341.56373255
		-H(Kcal/mol)	986278.406783	986278.172095356	986277.5320356	986276.8825633	986276.22367835
		-E(Kcal/mol)	986278.999152	986278.768229381	986412.5214834	986277.4987776	986276.84993283
	Cyclohexane ε =2.023	-G(Kcal/mol)	986338.160121	986338.532234161	986339.5431519	986340.5647374	986341.59699055
		-H(Kcal/mol)	986278.428119	986278.193430679	986277.5533709	986276.9038986	986276.24501368
		-E(Kcal/mol)	986279.020488	986278.789564704	986278.1595451	986277.5194854	986276.87126816

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

Medium	Dielectric constant (ε)	μ (Debye)
Gas	1	9.9948
Cyclohexane	2.023	12.7379
Benzene	2.247	12.9032
Ethanol	24.55	14.8415
DMSO	46.8	14.9741
Water	78.39	15.0369

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

Layer	Atom	Gas	Benzene	DMSO	Water	Cyclohexane	Ethanol
Layer 1	B34	0.812292	-0.79635	-0.79603	-0.79602	-0.79637	-0.79605
	B26	0.848251	-0.79719	-0.7969	-0.7969	-0.79722	-0.79692
	B35	0.786682	0.805621	0.802534	0.802444	0.80588	0.802721
	N38	-0.81384	0.777324	0.773288	0.773171	0.777686	0.77353
	B41	0.921925	-0.81292	-0.81206	-0.81203	-0.81299	-0.81211
	B36	0.781718	0.778762	0.771011	0.770783	0.779404	0.771482
Layer 2	N44	-0.45205	0.916218	0.91368	0.913563	0.916393	0.913866
	C48	0.435833	-0.42122	-0.41874	-0.41869	-0.42139	-0.41891
	O50	-0.42541	0.475104	0.484096	0.484346	0.474391	0.483509
Layer 3	N25	-0.79749	-0.81381	-0.81365	-0.81365	-0.81383	-0.81366
	B27	0.784503	0.84278	0.837056	0.836888	0.843241	0.837419
	N30	-0.82597	0.775183	0.763056	0.762695	0.776147	0.763836
	N32	-0.79656	-0.82514	-0.82449	-0.82446	-0.82519	-0.82453
	B26	0.848251	-0.79719	-0.7969	-0.7969	-0.79722	-0.79692
Layer 4	B15	0.785292	0.778691	0.76991	0.769647	0.779379	0.770476
	N8	-0.54115	-0.5404	-0.53831	-0.53825	-0.54058	-0.53843
	N23	-0.81384	0.778691	0.76991	0.769647	0.779379	0.770476
	B14	0.796561	0.791304	0.784353	0.784144	0.791846	0.784799
	N9	-0.54561	-0.54385	-0.54128	-0.54121	-0.54407	-0.54143
	B3	0.924982	0.923258	0.921182	0.921111	0.92341	0.921305
	N1	-0.44838	-0.44854	-0.44817	-0.44816	-0.44858	-0.44817

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

	Gas phase					Water				
Atom	***σ iso***	***σaniso***	***δ***	***Δσ***	***η***	***σ iso***	***σaniso***	***δ***	***Δσ***	***η***
N1	205.2212	51.3516	51.3516	51.3517	0.05375751	203.6597	49.6387	-36.201	49.6388	0.05929337
B3	99.8502	26.1219	17.4145	26.12185	0.01704297	99.7525	99.7525	17.4631	26.1946	0.01758616
C6	16.5448	140.8158	93.8772	140.8158	0.1019466	15.7857	138.3514	92.2343	138.3515	0.1072762
N8	194.1503	60.0747	-46.3562	60.0747	0.07417274	194.6425	59.9341	-46.1259	59.93415	0.0788816
N9	185.8593	73.7298	-52.4482	73.7298	0.07851162	185.6629	72.8467	-51.9632	72.8467	0.08350673

Table 4. Contd.

B14	98.1862	31.8245	21.2163	31.82445	0.0147917	97.9437	32.0367	21.3577	32.03665	0.01471346
B15	97.3265	29.9279	-25.2423	29.92795	0.04300384	97.4274	30.2824	-25.1524	30.2824	0.04542717
N23	145.4663	153.7932	102.5288	153.7933	0.07923317	145.3826	151.9511	101.3008	151.9511	0.08521995
N25	138.6591	124.2298	-95.504	124.2298	0.1523779	138.5064	123.4186	-95.3406	123.4187	0.1635112
B26	95.4217	24.6611	16.4407	24.661	0.01693832	95.3621	24.4943	16.3295	24.4942	0.01873584
B27	91.1146	37.3643	24.9095	37.36425	0.03447538	91.2645	37.4448	24.9632	37.4448	0.03735645
N30	160.874	159.0736	106.0491	159.0736	0.02424199	161.6092	157.3774	104.9182	157.3774	0.02694217
N32	137.6093	125.4131	-95.12	125.4132	0.1501851	137.0768	123.333	-95.0922	123.333	0.1628479
B34	98.3457	31.2758	20.8505	31.2758	0.005891273	98.0419	31.8994	21.2663	31.89945	0.01136999
B35	91.0759	37.2111	24.8074	37.21115	0.03401538	91.2616	37.0357	-24.8027	37.03565	0.03758105
B36	97.1876	28.4725	-25.71	28.4724	0.04568793	97.1533	29.2091	-25.6985	29.20905	0.04815386
N38	145.8798	154.8399	103.2266	154.8399	0.08599162	145.4821	154.4838	102.9892	154.4839	0.09063939
B41	101.5787	25.6497	-17.3573	25.6497	0.0248096	101.0145	25.2621	16.8414	25.2621	0.02273998
N44	209.343	51.8383	-38.3068	51.8383	0.05923216	208.2375	54.0932	36.0622	54.09325	0.05140984
C48	8.8502	145.4784	96.9856	145.4784	0.1075887	16.6962	144.5175	96.3449	144.5174	0.1139841
O50	-345.4604	1064.9991	709.9994	1064.999	0.8030118	-303.3762	994.4468	662.9645	994.4467	0.7134163

	DMSO					Benzene				
Atoms	***σ iso***	***σaniso***	***δ***	***Δσ***	***η***	***σ iso***	***σaniso***	***δ***	***Δσ***	***η***
N1	203.6917	49.6689	-36.2	49.7	0.0593	204.647	50.6902	-36.1047	50.7	0.0584
B3	99.7548	26.1935	17.4623	26.2	0.0176	99.8288	26.1582	17.4388	26.2	0.0180
C6	15.804	138.3981	92.2654	138	0.107E	16.267	139.8945	93.263	140	0.109
N8	194.6356	59.934	-46.1276	5.99	0.0789	194.4222	59.8946	-46.2133	59.9	0.0799
N9	185.6707	72.8673	-51.9699	72.9	0.0835	185.9215	73.3429	-52.1997	73.3	0.0844
B14	97.9487	32.0328	21.3552	32	0.0147	98.1029	31.9067	21.2711	31.9	0.0153
B15	97.4257	30.2756	-25.1526	30.3	0.0455	97.3649	30.059	-25.1562	30.1	0.0461
N23	145.3869	151.975	101.3167	152	0.0852	145.5002	152.8788	101.9192	153	0.0858
N25	138.5109	123.4317	-95.3455	123	0.164	138.6748	123.8234	-95.4658	124	0.165
B26	95.364	24.4954	16.3303	24.5	0.0187	95.4224	24.5189	16.3459	24.5	0.0190
B27	91.2624	37.4428	24.9619	37.4	0.0374	91.1811	37.3938	24.9292	37.4	0.0377
N30	161.6014	157.3959	104.9306	157	0.0269	161.2901	158.0438	105.3625	158	0.0271
N32	137.0887	123.3496	-95.0968	123	0.163	137.5058	123.8768	-95.2689	124	0.164
B34	98.0435	31.8989	21.266	31.9	0.0113	98.1128	31.866	21.244	31.9	0.0107
B35	91.2601	37.0388	-24.804	37	0.0376	91.1939	37.1582	-24.8777	37.2	0.0380
B36	97.1565	29.208	-25.6932	29.2	0.0482	97.2667	29.1621	-25.5752	29.2	0.0482
N38	145.4925	154.5057	103.0037	155	0.0907	145.7542	155.2268	103.4845	155	0.0915

Table 4. Contd.

B41	101.0119	25.2607	16.8405	25.3	0.0227	100.9629	25.2337	16.8225	25.2	0.0224
N44	208.2634	54.1266	36.0844	54.1	0.0515	209.1167	55.186	36.7906	55.2	0.0531
C48	16.7457	144.4291	96.286	144	0.114	17.9135	142.1492	94.7661	142	0.119
O50	-303.1195	994.0766	662.7178	994	0.713	-297.1894	985.9879	657.3253	986	0.706
			Cyclohexane					**Ethanol**		
Atoms	***σ iso***	***σaniso***	***δ***	***Δσ***	***η***	***σ iso***	***σaniso***	***δ***	***Δσ***	***η***
N1	204.7253	50.7732	-36.0936	50.8	0.05.84	203.7507	49.7335	-36.1952	49.7	0.0592
B3	99.834	26.1557	17.4372	26.2	0.0180	99.7596	26.1912	17.4607	26.2	0.0176
C6	16.2999	140.0171	93.3448	140	0.110	15.8408	138.4956	92.3304	13.8	0.108
N8	194.4069	59.8922	-46.22	59.9	0.0799	194.6217	59.9318	-46.1335	59.9	0.0790
N9	185.9374	73.3837	-52.2194	73.4	0.0845	185.6847	72.8996	-51.9845	72.9	0.0836
B14	98.1149	31.8959	21.264	31.9	0.0153	97.9587	32.0247	21.3498	32.0	0.0148
B15	97.3596	30.042	-25.1559	30.0	0.0461	97.4224	30.2609	-25.1532	30.3	0.0455
N23	145.5082	152.9537	101.9691	153	0.0858	145.3956	152.0338	101.3558	152	0.0853
N25	138.6877	123.8527	-95.4743	124	0.165	138.5219	123.4589	-95.354	123	0.164
B26	95.4269	24.5202	16.3468	24.5	0.0190	95.3681	24.4967	16.3311	24.5	0.0188
B27	91.1742	37.3905	24.9269	37.4	0.0378	91.2579	37.4396	24.9597	37.4	0.0374
N30	161.2632	158.0975	105.3983	158	0.0271	161.5839	157.4362	104.9575	157	0.0270
N32	137.5415	123.9205	-95.2857	124	0.164	137.1152	123.3798	-95.1051	123	0.163
B34	98.1202	31.8613	21.2408	31.9	0.0106	98.0472	31.8984	21.2656	31.9	0.0113
B35	91.1867	37.1667	-24.8843	37.2	0.0380	91.2571	37.0472	-24.8098	37.0	0.0376
B36	97.2743	29.1577	-25.5657	29.2	0.0482	97.1641	29.2062	-25.6852	29.2	0.0482
N38	145.7751	155.2875	103.5251	155	0.0916	145.5096	154.5527	103.0351	155	0.0907
B41	100.957	25.2337	16.8225	25.2	0.0224	101.0118	25.255	16.8362	25.3	0.0227
N44	209.1789	55.2595	36.8396	55.3	0.0533	208.3245	54.1931	36.1287	54.2	0.0516
C48	17.9971	141.9686	94.6457	142	0.119	16.8283	144.2606	96.1737	14.4	0.114
O50	-296.7189	985.3377	656.8918	985	0.706	-302.727	993.5176	662.345	994	0.713

pharmacology and drug delivery instead of the other nanocompounds.

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