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# Molecular Design and Theoretical Study on Novel High-nitrogen Energetic Azido Compounds

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**Abstract:** Seven high-nitrogen energetic compounds were devised:  $C(N_3)_4$ ,  $B(N_3)_3$ ,  $N(N_3)_3$ ;  $CC(N_3)_4$ ,  $BN(N_3)_4$ ,  $NN(N_3)_4$  and  $CC(N_3)_6$ , which are structurally similar to  $CH_4$ ,  $BH_3$ ,  $NH_3$  and  $C_2H_4$ . The molecular geometries, IR spectra, bond order and frontier orbital energies of these compounds were obtained at B3PW91/6-311 + G(d) level of theory. The calculated results show that they were stable on the related potential energy surface. The theoretical spectrum agreed well with the experimental value. According to the results of bond orders, we could predict that the possible primary decomposition reactions of the title compounds may be the elimination of azido group or the center bond breaking. The heat of formation, density and detonation performance of the above compounds were obtained. These results indicate that almost all titled compounds have potential applications in the field of high energy density materials.

**Key words:** physical chemistry; azide compound; high nitrogen compound; heat of formation; detonation velocity; detonation pressure

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## 1 Introduction

Scientists have been interested in compounds with high nitrogen content and even polynitrogen compounds (containing only nitrogen atoms) because of their potential applications as high-energy-density materials (HEDMs) in propulsion and explosive fields. High-nitrogen energetic compounds are also considered as "green" energetic materials owing to the relative stability of nitrogen as a reaction product. For the significant difference in bond energy between nitrogen atoms, these compounds have high energy content. In general, every azido group adds about 292.6 kJ to energy contents of the molecule, thus synthesis of molecules with a high number of azido groups is a useful as well as challenging way to synthesize high nitrogen energetic compounds<sup>[1]</sup>. There have been many experimental and theoretical studies on azido derivatives, and the results also indicates a good group additive effect on the detonation properties and supports the notion that introducing more azide substituents into the molecule increases its detonation performance<sup>[2-4]</sup>. Numerous homologous azides of the type  $M(N_3)_n$  ( $M$  = elements in groups 3 and 13 ( $n = 3$ ) and in groups 4 and 14 ( $n = 4$ )) as well as derivable salts have been studied in detail<sup>[5-6]</sup>. Some of them have been prepared and characterized to investigate the properties of highly energetic materials<sup>[7-8]</sup>. Polynitrogen compounds have caught increasing theoretical and empirical attention. The synthesis of such compounds involves great technical difficulties because these new chemical substances have no analogs under terrestrial conditions. Two hundred years of research have produced only a handful of synthesized all-nitrogen molecules and ions, however, a lot of stable  $N_n$  candidates are waiting to be detected<sup>[9-10]</sup>.

For great difficulties in the synthesis of such molecules, it is necessary to continue to design and develop new azido

HEDMs by theoretical computations in order to meet the continuing demand for improved energetic materials. Herein, seven novel azide compounds were devised and optimized:  $C(N_3)_4$ ,  $B(N_3)_3$ ,  $N(N_3)_3$ ;  $CC(N_3)_4$ ,  $BN(N_3)_4$ ,  $NN(N_3)_4$  and  $CC(N_3)_6$ . The results provide useful information for the molecular design of novel HEDMs.

## 2 Computational methods

All calculations were performed using the Gaussian 03 program<sup>[11]</sup>.

Structures of seven molecular were fully optimized using the density functional theory (DFT, B3PW91) framework<sup>[12]</sup> with the 6-311 + G(d) basis set. The Wiberg bond orders analysis<sup>[13]</sup>, harmonic vibrational frequencies, thermodynamic properties and detonation performance were calculated for the optimized structures at the same level. We have checked the B—N bonds of  $B(N_3)_3$  with the MP2 method.

The theoretical heat of formation was calculated with the following formulas<sup>[14]</sup>:

$$\Delta_f H^0(M, 0 \text{ K}) = \sum_{\text{atoms}} x \Delta_f H^0(X, 0 \text{ K}) - \left[ \sum_{\text{atoms}} x \varepsilon_0(X) - \varepsilon_0(M) - \varepsilon_{ZPE}(M) \right]$$

$$\Delta_f H^0(M, 298.15 \text{ K}) = \Delta_f H^0(M, 0 \text{ K}) + (H_M^0(298.15 \text{ K}) - H_M^0(0 \text{ K})) - \sum_{\text{atoms}} x (H_X^0(298.15 \text{ K}) - H_X^0(0 \text{ K}))$$

Where  $M$  denotes the molecule,  $X$  represents each element making up  $M$ ,  $x$  is the number of atoms of  $X$  in  $M$ ,  $\varepsilon_0(M)$  is the total energy of the molecule, and  $\varepsilon_{ZPE}(M)$  is its zero-point energy.  $H_M^0(298.15 \text{ K}) - H_M^0(0 \text{ K})$  and  $H_X^0(298.15 \text{ K}) - H_X^0(0 \text{ K})$  are enthalpy corrections for the molecule and atomic elements, respectively. The latter can be obtained from both calculated and experimental data<sup>[15]</sup>.

The density ( $\rho$ ,  $g \cdot cm^{-3}$ ) was predicted from the molecular volume, which was obtained from the statistical average of 100 single-point calculations for the optimized structure. The molar volume was defined as the space within a contour of density 0.001 e/Bohr<sup>3</sup> that was evaluated using Monte

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Carlo integration<sup>[16]</sup>.

Detonation velocity ( $D$ ,  $\text{km} \cdot \text{s}^{-1}$ ), and detonation pressure ( $p$ , GPa) can be predicted using the modified nitrogen equivalent (MNE)<sup>[17]</sup> as follows:

$$D = (690 + 1160\rho_0) \sum N^w$$

$$p = 1160(\rho_0 \sum N^w)^2 - 8.40$$

$$\sum N^w = \frac{100}{m} (\sum P_i N_{P_i} + \sum B_k N_{B_k} + \sum G_j N_{G_j})$$

Where  $\sum N^w$  is the corrected nitrogen equivalent of explosive,  $P_i$  is the molar number of gaseous detonation products per gram of explosive,  $N_{P_i}$ ,  $N_{B_k}$  and  $N_{G_j}$  are the coefficient of correct nitrogen equivalent for products, bond and group, respectively. The data come from the literatures<sup>[17]</sup>.  $B_k$  and  $G_j$  are the number of each kind of the bond and group in the molecular.

### 3 Results and discussion

#### 3.1 Molecular geometry

Fig. 1 shows the geometric structures, structural data and atomic numbering of the seven title compounds at the B3PW91/6-311 + G(d) level of theory.

The  $\text{B}(\text{N}_3)_3$  molecule with B—N bonds was also calculated with the MP2 method. In general, the typical bond length of N—N, N=N, N≡N; C—N, C=N and B—N is 1.450, 1.250, 1.100; 1.472, 1.287 and 1.465 Å<sup>[18-19]</sup>, respectively. For these compounds, all the bond lengths are close to typical bond data which indicate the bond length is reasonable and error of the theory calculation is acceptable. The bond angles for N(3)—C(1)—N(4) is 113.20° in  $\text{C}(\text{N}_3)_4$ , which is close to 109.28°, reflecting a tetrahedral configuration of the molecular and the  $sp^3$  orbital hybridization for the C(1) atoms. The bond angle for N(5)—N(1)—N(2) in  $\text{N}(\text{N}_3)_4$  is 105.47°. Owing to the impact of lone pair electrons, an almost pyramid configuration appears and the nonequivalent  $sp^3$  hybridization of atomic orbitals on N(1),

which is the same to  $\text{NH}_3$ . The bond angles for N(2)—B(1)—N(5) in  $\text{B}(\text{N}_3)_3$  is 119.99°, which is close to 120.00°, performing an plane triangle configuration and the  $sp^2$  orbital hybridization for the B(1) atoms just like the B atom in the  $\text{BH}_3$ . The dihedral angles of the this compound are nearly 0, which also clearly indicate that the  $\text{B}(\text{N}_3)_3$  is practically planar. The MP2/6-311 + G(d) results in brackets are in substantial agreement with the B3PW91 data, while the bond angles are determined to be much larger and the bond lengths are smaller by the MP2 calculation. The MP2 calculation finds that 120° of N—B—N angles is a more reasonable value. The bond angles for N(4)—M—N(3) and the dihedral angles in  $\text{CC}(\text{N}_3)_4$ ,  $\text{BN}(\text{N}_3)_4$  and  $\text{NN}(\text{N}_3)_4$  reflect the  $sp^2$  orbital hybridization for the center C, B and N atoms. Both of the two center C atoms in  $\text{CC}(\text{N}_3)_6$  take the  $sp^3$  hybridization, but the structure do not have any symmetric properties.

#### 3.2 Vibrational frequencies

The harmonic vibrational frequencies and their IR intensity for the seven title compounds were predicted at the B3PW91/6-311 + G(d) level. The IR spectra of the compounds are shown in Fig. 2, which shows the vibrational frequencies and their IR intensities for stationary points. The results show that the IR characters are very similar. Thus, it might be impossible to use IR to distinguish resembling compounds.

Vibrational frequencies of  $\text{B}(\text{N}_3)_3$  were also calculated at the MP2 level of theory. Table 1 shows the major frequencies and IR intensities calculated at the B3PW91 and MP2 levels, based on analogous geometry optimizations. The B3PW91 results match with the experimental spectrum<sup>[20]</sup>. Frequencies calculated with the MP2 method and corrected are better coincided with the experimental results than that with the B3PW91 method, indicating DFT calculations can provide a remarkably good description of the molecular, which also demonstrating that the dispersion and polarization function is applicable to azide compounds.

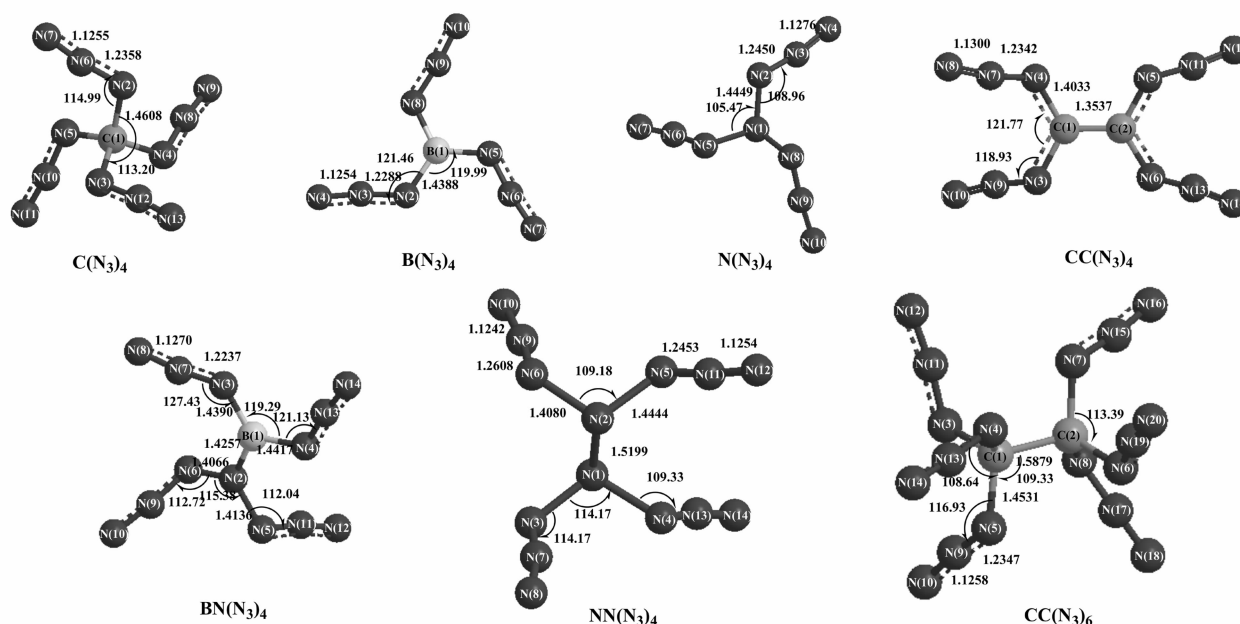


Fig. 1 Atomic numbering and optimized geometries of title compounds (Bond lengths are in Å, and bond angles are in degrees. The number in brackets is MP2 value)

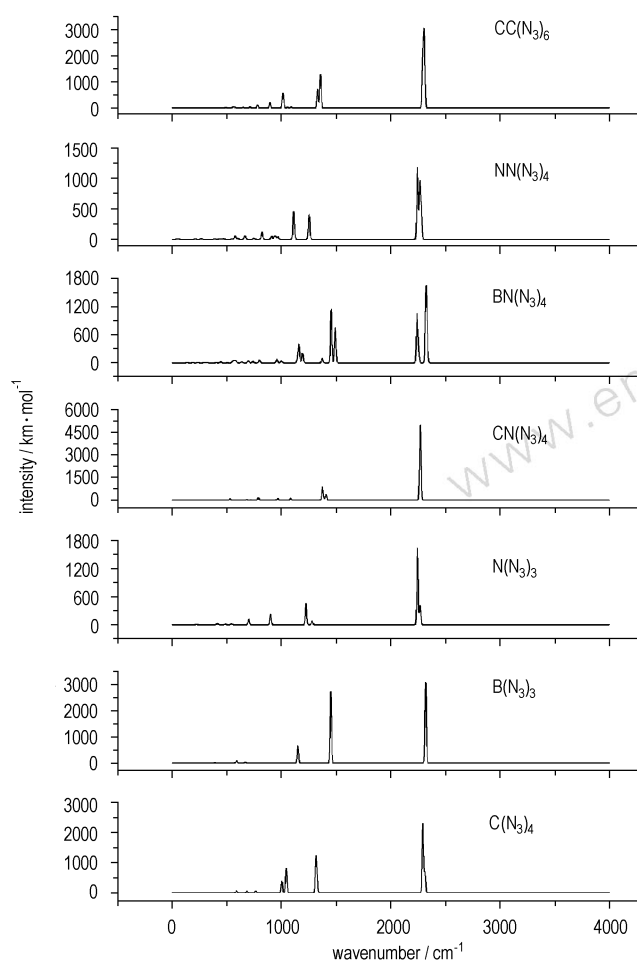


Fig. 2 IR spectra of the title compounds at B3PW91/6-311 + G(d) level

The absence of any imaginary frequency in the calculated results indicates that the optimized structures correspond to a minimum point on the potential energy surface. We assigned the main vibrational frequencies. The most intense vibrations in the IR spectrum are azide asymmetric vibrations at  $2243 \sim 2322 \text{ cm}^{-1}$  as well as N—C—N deformation vibrations ( $\delta_s$  and  $\delta_{as}$ ). Azide symmetric vibrations are evident at  $1316 \sim 1452 \text{ cm}^{-1}$ . N—C—N asymmetric vibrations are evident at  $1015 \sim 1374 \text{ cm}^{-1}$  in the  $C(N_3)_4$ ,  $CC(N_3)_4$  and  $CC(N_3)_6$ . N—B—N symmetric vibrations with a broad signal at  $1149$  and  $1151 \text{ cm}^{-1}$ , asymmetric vibrations with a broad signal at  $1451$  and  $1456 \text{ cm}^{-1}$ , respectively.  $930 \text{ cm}^{-1}$  and  $1160 \text{ cm}^{-1}$  are the N—N—N (the center N atom and two azido N atoms) asymmetric vibrations in the spectrum of  $N(N_3)_3$  and  $BN(N_3)_4$ .  $823 \text{ cm}^{-1}$  is the N—N—N (the two center N atoms and azido N atom) symmetric vibrations in the spectrum of  $NN(N_3)_4$ . At lower frequency mainly deformation and out-of-plane vibrations are observed.

Table 1 The major frequencies (IR intensities) of the  $B(N_3)_3$  molecule

calculated frequencies	B3PW91/6-311 + G(d)	MP2/6-311 + G(d)	experiment
$\nu_s(\text{N—B—N})$	1106(216)	1151(217)	1100
$\nu_s(\text{—N}_3)$	1395(947)	1453(948)	1360
$\nu_s(\text{—N}\equiv\text{N})$	2228(1065)	2318(1068)	2163

### 3.3 Wiberg bond orders and bond dissociation energies (BDEs)

The calculated Wiberg bond orders for title compounds are compared in Table 2. The Wiberg bond indices of all N—N bonds in the front of azido group for each compound are from 1.4028 to 1.4921, which are between the standard values of single bond (1.0) and double bonds (2.0). The values of the calculated bond order of the N—N bond at the end of the azido group are the highest, so the bond is the strongest, which is agree with the structure character of azido at the end of titled molecules. The table shows that the lowest index is at the bond between the center atom and the atom of azido group in the  $C(N_3)_4$ ,  $B(N_3)_3$ ,  $N(N_3)_3$ ,  $CC(N_3)_4$  and  $BN(N_3)_4$ , while the bond N(1)—N(2) and C(1)—C(2) between the center atoms in  $NN(N_3)_4$  and  $CC(N_3)_6$ , thus those bonds will be the weakest bond. From the above analysis we may predict that the elimination of azido group or the center bond breaking is the possible primary decomposition reaction of the title compounds.

In order to discuss the difficulty level of substitution sufficiently, dissociation energies of characteristic chemical bonds are calculated, comparing the fracture energies, experiments could be better guided. BDE could also provide us with information about the stability of compounds. The higher the BDE is, the better of stability of molecular will be. The bond dissociation energies (BDEs) of title compounds are showed at Table 3. BDE1 means dissociation energy of each bond N—N at the end of molecular, and BDE2 stands for fracture energy of bond between N and central atom, for example C—N, B—N in  $C(N_3)_4$ ,  $B(N_3)_3$  respectively. While things are different in  $BN(N_3)_4$ , there are two kinds of BDE1 and BDE2, respectively.

It could be indicated from values of BEDs that they are stable materials. Besides, it can also be inferred that  $BDE1 > BDE2$ , which means the N—N bond at the end of the azide group is much more stable than bond between N and central atom. Thus we get the similar conclusion as the results of Wiberg orbital analysis, crack of the azide group is the most possible reaction in these kinds of compounds.

### 3.4 Frontier orbital energy levels and their gaps

The molecular frontier orbital energy levels and their gaps are contained in Table 4. The energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) can be used to determine the activity of a molecule due to intramolecular charge transfer, so the LUMO-HOMO energy gaps for  $C(N_3)_4$ ,  $B(N_3)_3$ ,  $N(N_3)_3$ ;  $CC(N_3)_4$ ,  $BN(N_3)_4$ ,  $NN(N_3)_4$  and  $CC(N_3)_6$  were calculated at the B3PW91/6-311 + G(d) level. It is obvious to see from Table 3, the frontier orbital energies differ from different compounds. The differences predict that the chemical activity of the title compounds decrease in the order:  $B(N_3)_3 > C(N_3)_4 > CC(N_3)_6 > NN(N_3)_4 > BN(N_3)_4 > N(N_3)_3 > CC(N_3)_4$ . The smaller the energy gap is, the easier electron transfer HOMO LUMO and the more sensitive of the energetic molecule.

### 3.5 Predicted density and detonation properties

Our predicted results of volume ( $V$ ), density ( $\rho$ ), standard heat of formation ( $\Delta_f H^\theta$ ), detonation velocity ( $D$ ) and detonation pressure ( $p$ ) for  $C(N_3)_4$ ,  $B(N_3)_3$ ,  $N(N_3)_3$ ;  $CC(N_3)_4$ ,  $BN(N_3)_4$ ,  $NN(N_3)_4$  and  $CC(N_3)_6$  are listed in Table 5.

**Table 2** The Wiberg bond index at B3PW91/6-311 + G(d) level

species	bond	Wiberg bond order
$C(N_3)_4$	C(1)—N(2), C(1)—N(3), C(1)—N(4), C(1)—N(5)	0.9504
	N(3)—N(12), N(2)—N(6), N(4)—N(8), N(5)—N(10)	1.4515
	N(6)—N(7), N(12)—N(13), N(8)—N(9), N(10)—N(11)	2.4043
$B(N_3)_3$	B(1)—N(2), B(1)—N(5), B(1)—N(8)	0.9691
	N(2)—N(3), N(5)—N(6), N(8)—N(9)	1.4775
	N(3)—N(4), N(6)—N(7), N(9)—N(10)	2.3943
$N(N_3)_3$	N(1)—N(2), N(1)—N(5), N(1)—N(8)	0.9612
	N(2)—N(3), N(5)—N(6), N(8)—N(9)	1.4534
	N(3)—N(4), N(6)—N(7), N(9)—N(10)	2.3937
$CC(N_3)_4$	C(1)—C(2)	1.5594
	C(1)—N(3), C(1)—N(4), C(2)—N(5), C(2)—N(6)	1.0505
	N(3)—N(9), N(4)—N(7), N(5)—N(11), N(6)—N(13)	1.4593
	N(7)—N(8), N(11)—N(12), N(9)—N(10), N(13)—N(14)	2.3634
$BN(N_3)_4$	B(1)—N(2), B(1)—N(3), B(1)—N(4)	0.9808, 0.9671, 0.9559
	N(2)—N(5), N(2)—N(6)	0.9845, 0.9977
	N(3)—N(7), N(4)—N(13), N(5)—N(11), N(6)—N(9)	1.4231 ~ 1.4921
	N(7)—N(8), N(9)—N(10), N(11)—N(12), N(13)—N(14)	2.3721 ~ 2.4175
$NN(N_3)_4$	N(1)—N(2)	0.8807
	N(1)—N(3), N(2)—N(6)	1.0351
	N(1)—N(4), N(2)—N(5)	0.9637
	N(3)—N(7), N(6)—N(9)	1.4028
	N(4)—N(13), N(5)—N(11)	1.4381
	N(13)—N(14), N(11)—N(12)	2.4123
$CC(N_3)_6$	N(7)—N(8), N(9)—N(10)	2.4278
	C(1)—C(2)	0.8710
	C(1)—N(3), C(2)—N(6), C(1)—N(4), C(2)—N(7), C(1)—N(5), C(2)—N(8)	0.9545 ~ 0.9674
	N(3)—N(11), N(4)—N(13), N(5)—N(9), N(6)—N(19), N(7)—N(15), N(8)—N(17)	1.4577 ~ 1.4537
	N(13)—N(14), N(11)—N(12), N(9)—N(10), N(15)—N(16), N(19)—N(20), N(17)—N(18)	2.3912 ~ 2.4004

**Table 3** The bond dissociation energies (BDEs) of title compounds at B3PW91/6-311 + G(d) level

species	$C(N_3)_4$	$B(N_3)_3$	$N(N_3)_3$	$CC(N_3)_4$	$NN(N_3)_4$	$CC(N_3)_6$	$BN(N_3)_4$
$E_{BDE1}/\text{kJ} \cdot \text{mol}^{-1}$	562.76	768.86	414.14	710.92	436.33	757.80	759.24(B—N) 673.33(C—N)
$E_{BDE2}/\text{kJ} \cdot \text{mol}^{-1}$	-147.94	215.88	-208.97	-123.15	73.48	-221.28	209.16(B—N) -527.92(C—N)

**Table 4** The frontier orbital energies and their differences of title compounds at B3PW91/6-311 + G(d) level

species	$E_{LUMO}$	$E_{HOMO}$	$\Delta E_{LUMO-HOMO}$
$N(N_3)_3$	-281.7	-716.6	434.9
$B(N_3)_3$	-224.9	-799.9	575.0
$CC(N_3)_4$	-219.1	-617.9	398.8
$BN(N_3)_4$	-256.2	-722.6	466.4
$NN(N_3)_4$	-245.8	-737.1	491.3
$CC(N_3)_6$	-239.9	-774.5	534.5

The heat of formation for title compounds calculated at the B3PW91/6-311 + G(d) level. The heat of formation of the title compounds decrease in the order:  $CC(N_3)_6 > NN(N_3)_4 > CC(N_3)_4 > BN(N_3)_4 > C(N_3)_4 > N(N_3)_3 > B(N_3)_3$ .

The density, detonation velocity and detonation pressure results compared to experimental values for TNT ( $\rho = 1.600 \text{ g} \cdot \text{cm}^{-3}$ ,  $D = 6840 \text{ m} \cdot \text{s}^{-1}$ ,  $p = 20.3 \text{ GPa}$ ); RDX ( $\rho = 1.800 \text{ g} \cdot \text{cm}^{-3}$ ,  $D = 8750 \text{ m} \cdot \text{s}^{-1}$ ,  $p = 34.7 \text{ GPa}$ ) and HMX ( $\rho = 1.854 \text{ g} \cdot \text{cm}^{-3}$ ,  $D = 8917 \text{ m} \cdot \text{s}^{-1}$ ,  $p = 39.3 \text{ GPa}$ )<sup>[21]</sup>. The results reveal that those compounds are more powerful than TNT and comparable to RDX and HMX. Especially the  $C(N_3)_4$  and  $BN(N_3)_4$ , which is more powerful than the traditional high explosive HMX. It could also be seen from Table 5, the sequences of detonation the properties are as follows:  $D(C(N_3)_4) > D(BN(N_3)_4) > D>NN(N_3)_4 > D(CC(N_3)_6) > D(N(N_3)_3) > D(B(N_3)_3) > D(CC(N_3)_4)$ ,  $p(C(N_3)_4) > p(BN(N_3)_4) > p(CC(N_3)_6) > p>NN(N_3)_4 > p(B(N_3)_3) > p(N(N_3)_3) > p(CC(N_3)_4)$ , respectively. This indicates a good group additivity effect on the detonation properties. The more azido-groups, the higher

detonation velocity and detonation pressures values are.  $CC(N_3)_6$  and  $CC(N_3)_4$  special because that distance of C—C affects their densities. In this way, this result supports the

notion that introducing more azide substituents into a molecule increases its detonation performance. They would be novel potential HEDM candidates if successfully synthesized.

**Table 5** Density, heat of formation and detonation performance at B3PW91/6-311 + G(d) level

species	$C(N_3)_4$	$B(N_3)_3$	$N(N_3)_3$	$NN(N_3)_4$	$CC(N_3)_4$	$CC(N_3)_6$	$BN(N_3)_4$
molecular formula	$CN_{12}$	$BN_9$	$N_{10}$	$N_{14}$	$C_2N_{12}$	$C_2N_{18}$	$BN_{13}$
$M/g \cdot mol^{-1}$	180.13	136.90	140.10	196.14	192.14	276.2	192.94
$V/cm^3$	92.422	79.732	86.428	119.162	115.677	155.869	107.011
$\rho/g \cdot cm^{-3}$	1.949	1.717	1.621	1.646	1.661	1.772	1.803
$\Delta_f H^0/kJ \cdot mol^{-1}$ (0 K)	1355	682	1312	2703	2250	3241	2052
$\Delta_f H^0/kJ \cdot mol^{-1}$ (298 K)	1165	668	1295	2681	2233	3214	1849
$D/m \cdot s^{-1}$	9397	7957	9351	10419	9416	10062	9864
$p/GPa$	41.0	27.3	36.3	45.6	37.4	44.5	43.2

## 4 Conclusions

In our research, seven possible azide substituents were investigated using quantum chemical calculations. Some of the molecular geometries were determined for the first time. Results for harmonic vibrational frequencies reveal that the title compounds have a very stable structure, with a minimum on the potential energy surface and the absence of any negative mode. Wiberg bond orders analysis and BDE proved that the N—N bond at the end of the azide group is the strongest and the bond close to central atom is the weakest. The frontier orbital energies and their differences predict that chemical activity of the title compounds decrease as follows:  $B(N_3)_3 > C(N_3)_4 > CC(N_3)_6 > NN(N_3)_4 > BN(N_3)_4 > N(N_3)_3 > CC(N_3)_4$ . Calculations revealed that those compounds have relatively high detonation properties, which indicate that they might be HEDM candidates. This study provides some valuable information for the molecular design of novel HEDMs by exploring structural energetic properties.

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## 新型高氮含能叠氮化物的分子设计与理论研究

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**摘 要:** 根据  $\text{CH}_4$ 、 $\text{BH}_3$ 、 $\text{NH}_3$  以及  $\text{C}_2\text{H}_4$  的结构特点, 设计了 7 种新型叠氮类高氮含能化合物  $\text{C}(\text{N}_3)_4$ 、 $\text{B}(\text{N}_3)_3$  和  $\text{N}(\text{N}_3)_3$ ;  $\text{CC}(\text{N}_3)_4$ 、 $\text{BN}(\text{N}_3)_4$ 、 $\text{NN}(\text{N}_3)_4$  和  $\text{CC}(\text{N}_3)_6$ , 在 B3PW91/6-311 + G(d) 水平下对上述化合物进行了构型优化、振动频率以及键级分析, 计算结果表明, 所有化合物均无虚频, 为势能面上的稳定结构, 理论计算的红外结果与现有的实验结果十分相符。键级结果表明中心原子形成的键相对较弱, 为爆炸时可能的首发键。计算得到了目标化合物的生成热、密度、爆速和爆压。计算得到几乎所有分子的爆速和爆压都超过了 HMX, 在含能材料领域具有潜在的应用前景。

**关键词:** 物理化学; 叠氮化合物; 高氮化合物; 生成热; 爆速; 爆压

中图分类号: TJ55; O64

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### 第四届固体推进剂安全技术研讨会征文通知(第一轮)

第四届固体推进剂安全技术研讨会拟定于 2013 年 7 月下旬在安徽黄山召开, 此次会议由航天工业固体推进剂安全技术研究中心、华中危险化学品安全检测检验中心主办, 航天科技集团公司四院四十二所承办。

会议主题: 固体推进剂安全技术研究进展与发展方向

#### 一、征文范围

- |                         |                      |
|-------------------------|----------------------|
| (1) 固体推进剂安全技术研究进展       | (5) 固体推进剂安全性评估、评价方法  |
| (2) 固体推进剂配方与新型含能材料安全性   | (6) 火箭发动机、导弹武器安全评估技术 |
| (3) 固体推进剂安全性试验方法与测试技术   | (7) 火药、炸药及火工品安全技术    |
| (4) 固体推进剂安全性数值模拟及仿真分析技术 | (8) 危险化学品安全技术        |

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(1) 观点明确、数据可靠、图表清晰、文字简洁流畅(格式见附件); (2) 文责自负, 论文不应涉及他人知识产权, 须通过单位保密审查; (3) 投稿请注明作者姓名、单位、详细通讯地址、联系电话、传真、电子邮箱等; (4) 投稿请寄打印稿和电子文档各一份, 并附单位保密审查证明; (5) 录用稿件将统一编入《第四届固体推进剂安全技术研讨会论文集》, 创新性和高质量的论文将向《固体火箭技术》、《含能材料》等专业核心期刊推荐; (6) 本论文集已加入中国知网、万方数据资源系统数字化期刊群并全文入网, 如作者不同意论文编入数据库或入网, 请在投稿时声明。

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