

# Searching for a new family of insensitive high explosives by introducing N hybridization and N-oxides into a cage cubane

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**Abstract** A new family of energetic azacubane *N*-oxides were designed by introducing *N*-oxides into azacubanes and investigated by using density functional theory. Introducing the *N*-oxides into the azacubanes could improve their detonation performance significantly due to the increase of the OB and  $\rho$  but would also increase the sensitivity to some extent. These effects would be further enhanced as the numbers of *N*-oxides increase. Among all the designed azacubane *N*-oxides, D6-4 (1,3,5,7-tetraazacubane-1,3,5,7-tetraoxides) has higher detonation performance than one famous high explosive HMX (1,3,5,7-tetranitro-1,3,5,7-tetrazocane) and lower sensitivity than one very insensitive explosive TNT (1-methyl-2,4,6-trinitrobenzene), suggesting that its overall performance is outstanding and may be considered as the potential candidate of insensitive high explosives. The internal small cage C-N skeleton of D6-4 is surrounded by the external big cage hydrogen bonds and this special double cage structure may be an important reason why it has low sensitivity.

**Keywords** *N*-oxides · Azacubane · Cage · Density functional theory · Detonation performance

## Introduction

The introduction of *N*-oxides into energetic azacyclo compounds such as triazole and tetrazole has become a hot research area [1–10] since increasing oxygen balance and density can effectively improve the detonation performance and removing lone pair electron density can enhance the stability.

Göbel et al. [3] and Dippold et al. [4] synthesized the nitrogen-rich salts of nitrotetrazole-2*N*-oxides and 3,3'-dinitro-5,5'-bis-1,2,4-triazole-1,1'-diol, respectively and found that both of them have better detonation performance than corresponding compounds without *N*-oxides. Recently we [10] designed a novel powerful tetrazole *N*-oxide named 1-amino-5-nitrotetrazole-3*N*-oxide, which has both higher energetic performance than 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) and lower sensitivity than 1-methyl-2,4,6-trinitrobenzene (TNT). Although these investigations have been done on the *N*-oxides of nitrogen heterocycles, to our best knowledge, no work devoted to study the *N*-oxides of energetic caged compounds was done till now. Because of their obviously different structures, it may be expected that the effects of introducing *N*-oxides into energetic caged compounds on their structures and properties would be different from these effects in energetic azacyclo compounds. It is unclear whether the introduction of *N*-oxides into energetic caged compounds would obviously improve the explosive performance and stability. If so, a new development direction of explosives may come forth. Thus, it is needed to investigate the structures and properties of cage *N*-oxides compounds.

In the recent decades, theoretical studies based on quantum chemical treatment have gained acceptance as a useful and valuable research tool to screen the candidates of novel explosives with high energetic performance and reduced sensitivity, therefore avoiding a large amount of expensive, difficult and dangerous experimental tests. They are beneficial for learning the relationships between molecular structure and property, which in turn can help for designing better and more efficient laboratory tests. Hence, theoretical design of candidate compounds with high energy and low sensitivity is the primary step for synthesizing new improved explosives.

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In this work, we used a cubane as a base skeleton. Since the sensitivity of the energetic compounds with N-N single bonds would be very high, four series of azacubanes (Fig. 1) are designed by introducing one to four nitrogen atoms into the cubane, respectively. Then, four series of azacubane *N*-oxides (Fig. 2) are designed by the introduction of one to four *N*-oxides into the most stable compounds in each series of azacubanes. To decrease the synthesis risk and difficulty, here we do not introduce any nitro groups. Finally, the molecular geometry, heats of formation, energetic properties, and impact sensitivity of this new family of energetic compounds are investigated by using density functional theory (DFT).

### Computational method

The calculations of gas-phase heats of formation of azacubanes and azacubane *N*-oxides were carried out for the atomization reaction  $C_aH_bO_cN_d \rightarrow aC(g) + bH(g) + cO(g) + dN(g)$  by using the CBS-4M theory.

According to Hess's law of constant heat summation [11], the solid-phase heat of formation can be obtained from the gas-phase heat of formation ( $\Delta H_{f, \text{gas}}$ ) and heat of sublimation ( $\Delta H_{\text{sub}}$ ):

$$\Delta H_{f, \text{solid}} = \Delta H_{f, \text{gas}} - \Delta H_{\text{sub}} \quad (1)$$

Politzer et al. [12, 13] reported that the heat of sublimation correlates with the molecular surface area and the electrostatic

interaction index  $\nu\sigma_{\text{tot}}^2$  for energetic compounds. The empirical expression of the approach is as follows:

$$\Delta H_{\text{sub}} = aA^2 + b(\nu\sigma_{\text{tot}}^2)^{0.5} + c, \quad (2)$$

where  $A$  is the surface area of the 0.001 electrons·bohr<sup>-3</sup> isosurface of the electronic density of the molecule,  $\nu$  describes the extent of balance between positive potential and negative potential on the isosurface, and  $\sigma_{\text{tot}}^2$  is a measure of the variability of the electrostatic potential on the molecular surface. The coefficients  $a$ ,  $b$ , and  $c$  have been determined by Rice et al.:  $a=2.670 \times 10^{-4} \text{ kcal mol}^{-1} \text{ \AA}^{-4}$ ,  $b=1.650 \text{ kcal mol}^{-1}$ , and  $c=2.966 \text{ kcal mol}^{-1}$  [14]. The descriptors  $A$ ,  $\nu$ , and  $\sigma_{\text{tot}}^2$  were calculated by using the computational procedures proposed by Bulat et al. [15]. This approach has been demonstrated to predict reliably the heats of sublimation of many energetic organic compounds [15, 16]. These calculations were carried out at the B3LYP/6-311++G(2df,2p)/B3LYP/6-31G(d) level [13].

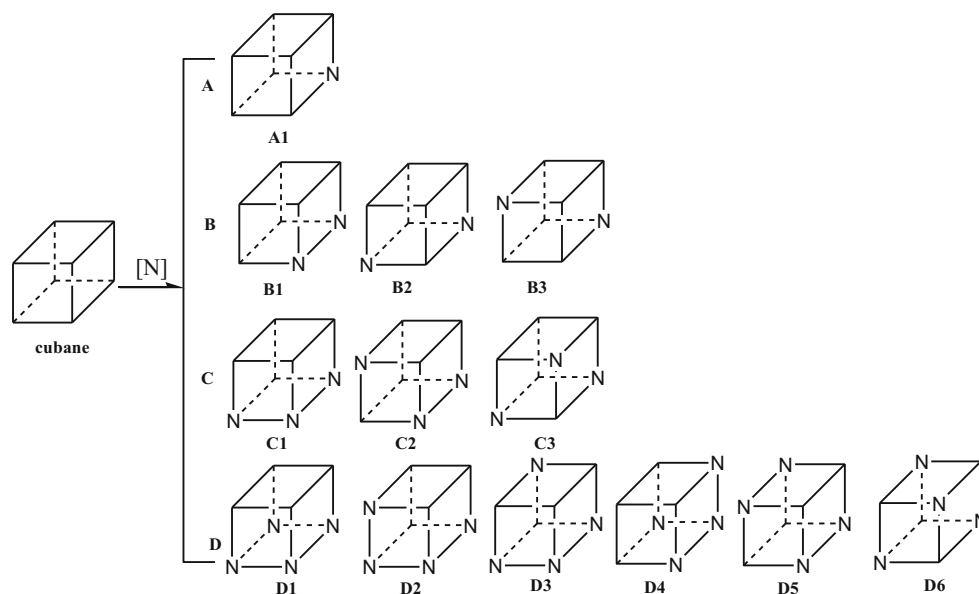
The detonation velocity and pressure were estimated by the Kamlet-Jacobs equations [17] as:

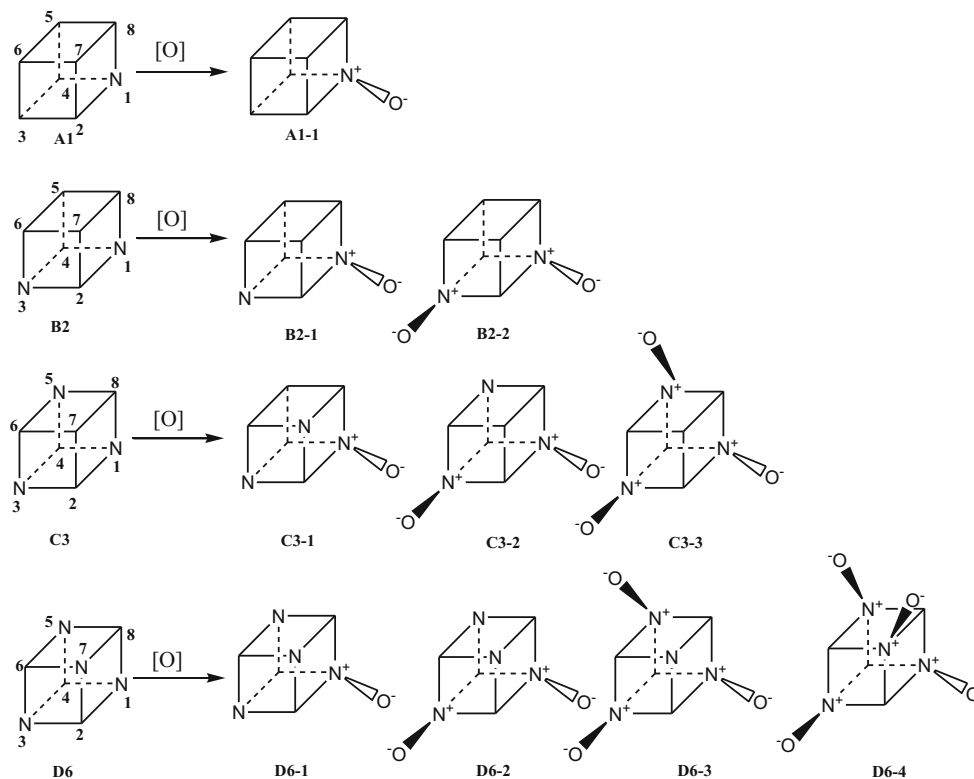
$$D = 1.01 \left( N\bar{M}^{1/2} Q^{1/2} \right)^{1/2} (1 + 1.30\rho) \quad (3)$$

$$P = 1.558\rho^2 N\bar{M}^{1/2} Q^{1/2}, \quad (4)$$

where each term in the equations of (1) and (2) is defined as follows:  $D$ , the detonation velocity (km/s);  $P$ , the detonation

**Fig. 1** Molecular frameworks of designed azacubanes



**Fig. 2** Molecular frameworks of designed azacubane *N*-oxides

pressure (GPa);  $N$ , the moles of detonation gases per gram explosive;  $\bar{M}$  the average molecular weight of these gases;  $Q$ , the heat of detonation (cal/g); and  $\rho$ , the loaded density of explosives ( $\text{g}/\text{cm}^3$ ). For known explosives, their  $Q$  and  $\rho$  can be measured experimentally; thus their  $D$  and  $P$  can be calculated according to Eq. 3 and Eq. 4. However, for some compounds, their  $Q$  and  $\rho$  cannot be evaluated from experimental measures. Therefore, to estimate their  $D$  and  $P$ , we first need to calculate their  $Q$  and  $\rho$ . The detonation products are supposed to be only  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ , and  $\text{N}_2$ , so released energy in the decomposition reaction reaches its maximum.

The theoretical density was obtained using an improved equation proposed by Politzer et al. [18], in which the interaction index  $\nu\sigma_{tot}^2$  was introduced:

$$\rho = \alpha \left( \frac{M}{V(0.001)} \right) + \beta\nu(\sigma_{tot}^2) + \gamma, \quad (5)$$

where  $M$  is the molecular mass ( $\text{g mol}^{-1}$ ) and  $V(0.001)$  is the volume of the 0.001 electrons/bohr<sup>3</sup> contour of electronic density of the molecule ( $\text{cm}^3/\text{molecule}$ ). The coefficients  $\alpha$ ,  $\beta$ , and  $\gamma$  are 0.9183, 0.0028, and 0.0443, respectively. These calculations were carried out at the density functional B3PW91/6-31G(d,p) level [18].

The free space per molecule in the unit cell, designated  $\Delta V$ , can be used to estimate the impact sensitivity of an energetic compound [19].  $\Delta V$  can be represented as the difference between the effective volume per molecule that would be required to completely fill the unit cell,  $V_{\text{eff}}$ , and the intrinsic gas phase molecular volume,  $V(0.003)$ :

$$\Delta V = V_{\text{eff}} - V_{\text{int}} = M/\rho - V(0.003), \quad (6)$$

**Table 1** Calculated total energies (a. u.) of four series of the azacubanes

Compound	Total energy
A1	-325.509178
B1	-341.514812
B2	-341.540112
B3	-341.535444
C1	-357.522703
C2	-357.543104
C3	-357.571855
D1	-373.505628
D2	-373.528019
D3	-373.552347
D4	-373.532562
D5	-373.548037
D6	-373.604144

**Table 2** Calculated bond lengths (Å) of A1, B2, C3, D6 and four series of the azacubane *N*-oxides

	N1-C2	C2-C3	C3-C4	C4-N1	C5-C6	C6-C7	C7-C8	C8-C5	N1-C8	C2-C7	C3-C6	C4-C5	N-O
A1	1.533	1.559	1.560	1.533	1.576	1.577	1.559	1.560	1.534	1.559	1.577	1.559	
A1-1	1.577	1.558	1.558	1.577	1.575	1.575	1.557	1.558	1.577	1.558	1.575	1.558	1.290
	N1-C2	C2-N3	N3-C4	C4-N1	C5-C6	C6-C7	C7-C8	C8-C5	N1-C8	C2-C7	N3-C6	C4-C5	N-O
B2	1.520	1.520	1.520	1.520	1.564	1.564	1.564	1.564	1.537	1.548	1.537	1.548	
B2-1	1.572	1.547	1.562	1.588	1.563	1.534	1.511	1.547	1.572	1.511	1.563	1.562	1.286
B2-2	1.562	1.562	1.563	1.562	1.561	1.561	1.561	1.561	1.590	1.543	1.590	1.543	1.287
	N1-C2	C2-N3	N3-C4	C4-N1	N5-C6	C6-C7	C7-C8	C8-N5	N1-C8	C2-C7	N3-C6	C4-N5	N-O
C3	1.508	1.508	1.524	1.524	1.553	1.524	1.524	1.553	1.524	1.508	1.524	1.553	
C3-1	1.515	1.578	1.567	1.500	1.522	1.552	1.551	1.515	1.579	1.551	1.522	1.500	1.283
C3-2	1.570	1.570	1.559	1.560	1.522	1.550	1.511	1.511	1.583	1.548	1.584	1.0489	1.282
C3-3	1.574	1.574	1.546	1.546	1.511	1.546	1.550	1.574	1.574	1.546	1.574	1.545	1.284
	N1-C2	C2-N3	N3-C4	C4-N1	N5-C6	C6-N7	N7-C8	C8-N5	N1-C8	C2-N7	N3-C6	C4-N5	N-O
D6	1.512	1.512	1.512	1.512	1.512	1.512	1.512	1.512	1.512	1.512	1.512	1.512	
D6-1	1.574	1.504	1.505	1.574	1.510	1.510	1.505	1.504	1.574	1.505	1.510	1.505	1.279
D6-2	1.566	1.566	1.566	1.566	1.502	1.502	1.502	1.502	1.578	1.495	1.578	1.495	1.277
D6-3	1.573	1.573	1.554	1.554	1.573	1.489	1.489	1.572	1.572	1.489	1.572	1.554	1.278
D6-4	1.557	1.557	1.558	1.557	1.557	1.557	1.557	1.557	1.557	1.557	1.558	1.557	1.281

where  $V(0.003)$  is defined as the volume enclosed by the 0.003 electrons/bohr<sup>3</sup> contour of the molecule's electronic density.  $M$  is the molecular mass and  $\rho$  is the crystal density. These calculations were carried out at the density functional B3PW91/6-31G(d,p) level [19].

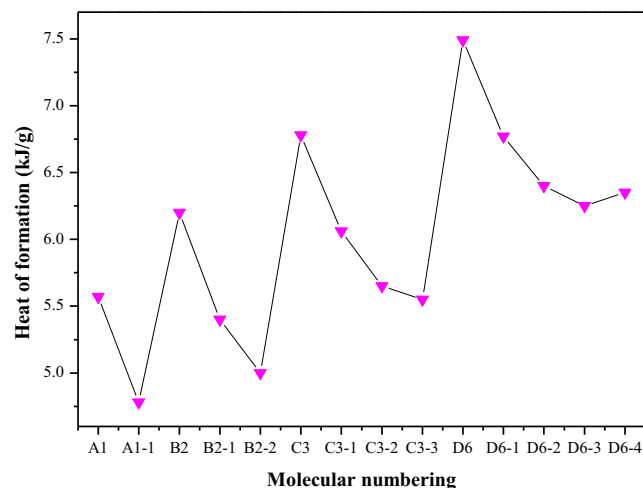
Other calculations were performed at the B3LYP/6-31+G(d,p) level with the Gaussian 03 package [20]. In the geometry optimization, the maximum force was converged less than 0.00045 eV/Å, the RMS force less than 0.0003 eV/Å, the maximum displacement less than 0.0018 Å, and the RMS displacement less than 0.0012 Å. All of the optimized structures were characterized to be true local energy minima on the potential energy surfaces without imaginary frequencies.

## Results and discussion

### Molecular geometry

Table 1 lists the calculated total energies of the designed four series of azacubanes. It is found that A1, B2, C3, and D6 have the lowest values in each series, indicating that they are the most stable compounds in series A, B, C, and D, respectively. Thus, A1, B2, C3, and D6 are used as the base skeleton and four series of azacubane *N*-oxides are designed by introducing one to four *N*-oxides into them, respectively, as depicted in Fig. 2. Their calculated bond lengths (Å) are listed in Table 2. Generally, in each series, the C-N bond lengths of azacubane *N*-oxides are longer than those of azacubanes. The

differences of the bond lengths of different C-N bonds in the former are much bigger than those in the later, suggesting that the introduction of *N*-oxides can reduce the structural symmetry and weaken the molecular stability, which is different from the case of azacyclo compounds and many of which are obviously stabilized by this. So it may be inferred that introducing *N*-oxides into azacubanes would increase the sensitivity. In addition, all the C-N bond lengths in D6-4 are very close to each other, which may suggest that it has good structural symmetry.



**Fig. 3** The calculated solid-phase heats of formation of the azacubanes and azacubane *N*-oxides

**Table 3** The densities ( $\rho$ , g/cm<sup>3</sup>),  $Q$  (kJ/g),  $D$  (km/s), and  $P$  (GPa) of D6-4, ONC, and HMX

Compound	$\rho$	$Q$	$D$	$P$
ONC	1.97 (1.98 <sup>a</sup> , 1.97 <sup>b</sup> )	8.2 (8.2 <sup>b</sup> )	9.6 (9.6 <sup>a</sup> )	43.6 (43.5 <sup>b</sup> )
D6-4	1.83	11.5	9.6	41.5
HMX	1.91 (1.90 <sup>c</sup> )	6.4 (6.3 <sup>d</sup> )	9.2 (9.1 <sup>c</sup> )	39.1 (39.0 <sup>c</sup> )

<sup>a</sup> Calculated values from ref. [21]. <sup>b, c, d</sup> Experimental values from ref. [26], [27], and [28], respectively

### Heats of formation and energetic properties

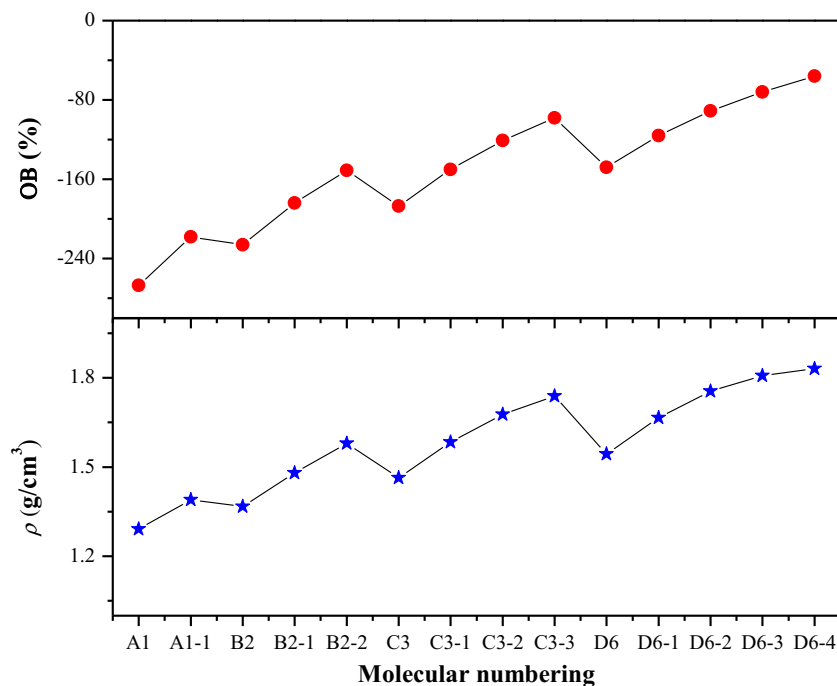
Figure 3 displays the calculated solid-phase heats of formation of the azacubanes and azacubane *N*-oxides. In each series, all of the azacubane *N*-oxides have lower heats of formation than the azacubanes. As the numbers of *N*-oxides increase, their heats of formation decrease gradually except for D6-4 and D6-3, indicating that introducing *N*-oxides into the azacubanes reduces the heats of formation and this effect is further enhanced when the numbers of *N*-oxides increase. The heats of formation of the azacubane *N*-oxides are above 4.7 kJ/g and eight of them have the heats of formation over 6.0 kJ/g, which are much higher than those of HMX (1,3,5,7-tetranitro-1,3,5,7-tetrazocane, 0.4 kJ/g, Table 3) [21] and ONC (1,2,3,4,5,6,7,8-octanitrocubane, 1.8 kJ/g, Table 3) [22], and even comparable with that of one nitrogen-high compound 1,1'-azobis(tetrazole) (6.2 kJ/g) [23] which has extremely high heat of formation. This shows that all the

azacubane *N*-oxides possess very high heats of formation and this is mainly derived from their original azacubane cage skeletons that contain very high energy.

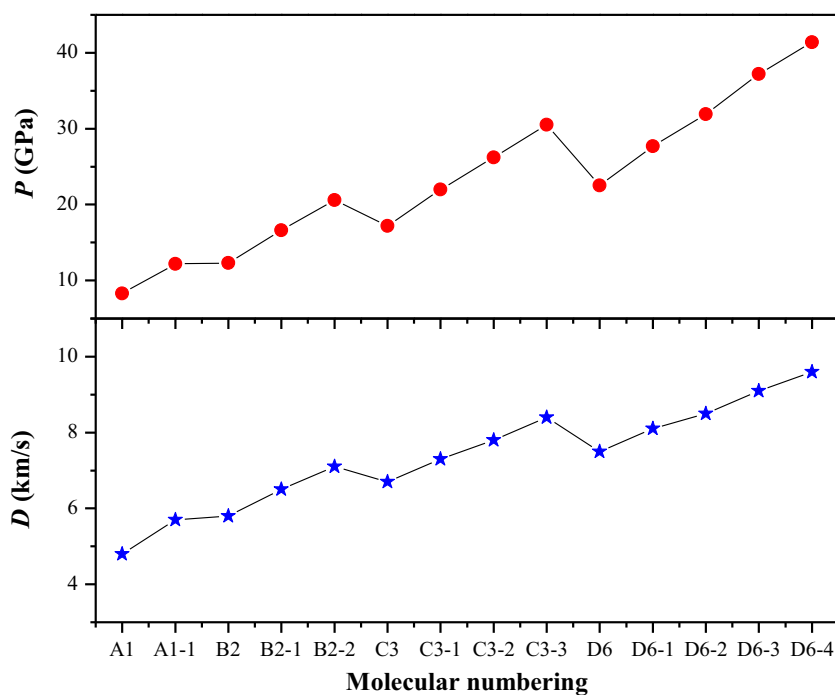
Oxygen balance (OB) and density ( $\rho$ ) are two important factors relevant to the detonation performance of energetic compounds. In general, the higher the oxygen balance and density, the larger the detonation velocity and pressure, and the better the performance of the explosive. Figure 4 depicts the calculated OB and  $\rho$  of the azacubanes and azacubane *N*-oxides. In each series, the azacubane *N*-oxides have higher OB and  $\rho$  than corresponding azacubanes. As the numbers of *N*-oxides increase, their OB and  $\rho$  increase dramatically, indicating that the introduction of *N*-oxides into azacubanes is a very effective way to enhance the OB and  $\rho$  of the azacubanes. Therefore, the explosive performance may be improved significantly by introducing the *N*-oxide.

Detonation velocity ( $D$ ) and detonation pressure ( $P$ ) are two of the most important parameters directly reflecting the performance of the explosives. Figure 5 displays the calculated  $D$  and  $P$  of the azacubanes and azacubane *N*-oxides. Since the OB and  $\rho$  of the azacubane *N*-oxides are obviously higher than those of corresponding azacubanes, the former have higher  $D$  and  $P$  than the later. In each series, the  $D$  and  $P$  of azacubane *N*-oxides are obviously improved with the increment of the numbers of *N*-oxides. In a word, introducing *N*-oxides into the azacubanes can markedly enhance the detonation performance due to the increase of their OB and  $\rho$ .

**Fig. 4** The calculated oxygen balance (OB) and density ( $\rho$ ) of the azacubanes and azacubane *N*-oxides

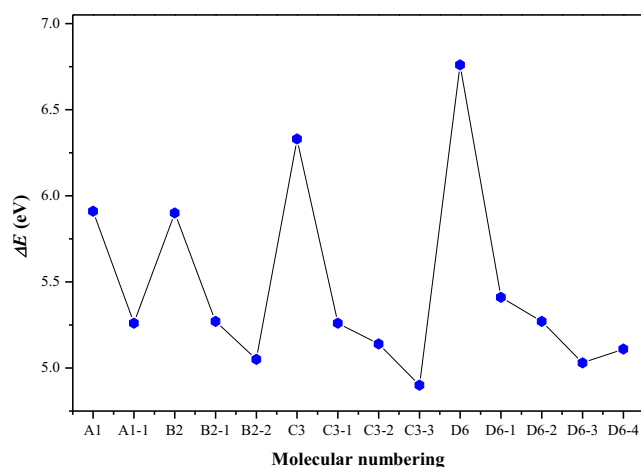


**Fig. 5** The calculated detonation velocity ( $D$ ) and detonation pressure ( $P$ ) of the azacubanes and azacubane  $N$ -oxides



### Sensitivity

Previous studies [24, 25] reported that for energetic compounds with similar structure or with similar thermal decomposition mechanism, the larger the HOMO-LUMO gap ( $\Delta E$ ) is, the more difficult the electron transfers from the valence band to the conduction band and the less they become decomposed and exploded. That is to say, for an explosive, a smaller value of  $\Delta E$  means a higher sensitivity. Figure 6 displays the calculated  $\Delta E$  values of azacubanes and azacubane  $N$ -oxides. It can be seen that azacubane  $N$ -oxides have lower  $\Delta E$  values than the corresponding azacubanes in each series, and  $\Delta E$  further decrease with the increasing of numbers of  $N$ -oxides except for D6-4, whose  $\Delta E$  values is



**Fig. 6** The calculated HOMO-LUMO gap ( $\Delta E$ ) values of the azacubanes and azacubane  $N$ -oxides

slightly higher than those of D6-3, which may be because D6-4 has better structural symmetry and more intramolecular hydrogen bonds than D6-3. In all, generally, the introduction of  $N$ -oxides into azacubanes would increase the sensitivity, and this effect can be further strengthened with the increment of numbers of  $N$ -oxides. Thus, introducing  $N$ -oxides more or less destabilizes the system.

The synthesis methods of azacubanes are being studied. Once the azacubanes could be synthesized, the  $N$ -oxides of azacubane would be synthesized successfully.

### Selection of insensitive high explosives

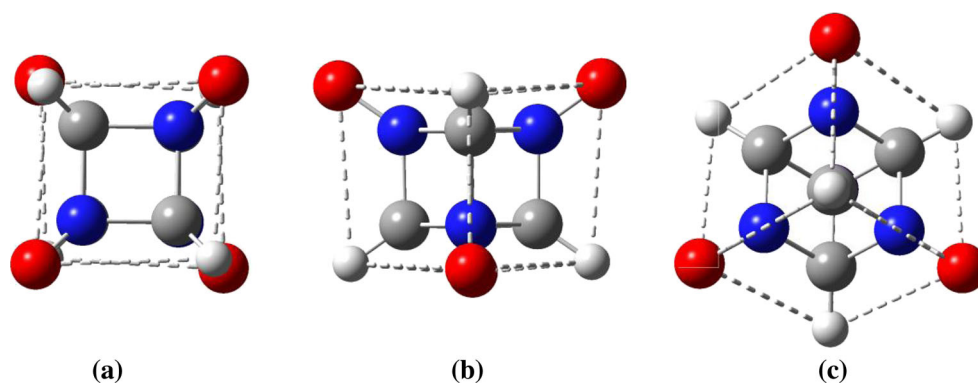
Among the azacubane  $N$ -oxides, it is found that D6-4 (1,3,5,7-tetraazacubane-1,3,5,7-tetraoxides) has the highest OB,  $\rho$ ,  $D$ , and  $P$ . For a comparison, Table 3 lists the  $\rho$ ,  $Q$ ,  $D$ , and  $P$  of D6-4, ONC, and HMX. Though D6-4 has lower  $\rho$  than HMX, its  $Q$  is far larger than that of HMX, making it have higher  $D$  and  $P$  than HMX. D6-4 has higher  $Q$  but lower  $\rho$  and  $P$  than ONC and its  $D$  is the same as that of ONC. In all, the detonation performance of D6-4 is between that of HMX and ONC, showing that D6-4 is very powerful.

**Table 4**  $\Delta V$  values of D6-4, TNT, LLM-105, and NTO

Compound	$\Delta V$ ( $\text{\AA}^3$ )
NTO	23 (21 <sup>a</sup> )
LLM-105	35 (35 <sup>a</sup> )
D6-4	36
TNT	59 (58 <sup>a</sup> )

<sup>a</sup> Calculated values from ref. [19]

**Fig. 7** (a) The optimized structures of D-4. (b) and (c) The perspective view of D-6 from other viewpoints. White, red, blue, and gray spheres stand for H, O, N, and C atoms, respectively. The hydrogen bonding is displayed as dotted lines



For an insensitive high explosive, both high energy and low sensitivity are required. The free space per molecule in the unit cell, designated  $\Delta V$ , can be used to estimate the impact sensitivity of an energetic compound [19]. Generally, the higher the  $\Delta V$  value is, the more sensitive the compound. Table 4 gives the  $\Delta V$  values of D6-4 and three insensitive explosives TNT, LLM-105 (2,6-diamino-3,5-dinitropyrazine-1-oxide), and NTO (3-nitro-1,2,4-triazole-5-one). From Table 4, it can be seen that the  $\Delta V$  values increase in the order of TNT, D6-4, LLM-105, and NTO, indicating that D6-4 is more sensitive than NTO and LLM-105 but more insensitive than TNT. This means that D6-4 is a very insensitive explosive. In all, D6-4 has higher detonation performance than HMX and lower sensitivity than TNT, suggesting that its overall performance is outstanding and it may be a very attractive candidate for experiments. Considering the detonation performance and sensitivity, D6-4 may be considered as the potential candidate of insensitive high explosives.

Figure 7 depicts the optimized structure of the derivative D6-4. Twelve intramolecular hydrogen bonds are formed between the four oxygen atoms and four hydrogen atoms and it looks like that the internal small cage C-N skeleton is surrounded by the external big cage hydrogen bonds. This special double cage structure is obviously different from any other known energetic compounds and may be an important reason why D6-4 is very insensitive though it even has higher detonation performance than HMX.

## Conclusions

In this work, we used a cubane as a base skeleton to design a new family of energetic azacubane *N*-oxides and investigate the effects of N hybridization and *N*-oxide on their structures and properties by using the DFT method. The results indicate that introducing the *N*-oxides into the azacubanes slightly reduces the heats of formation but markedly enhances the detonation performance due to the increase of the OB and  $\rho$ . All of these effects can be further enhanced as the numbers of

the *N*-oxides increase. Among four series of the azacubane *N*-oxides, D6-4 (1,3,5,7-tetraazacubane-1,3,5,7-tetraoxides) has higher energetic performance than HMX and lower sensitivity than TNT, suggesting that its overall performance is outstanding and may be considered as the potential candidate of insensitive high explosives. The special double cage structure of D6-4 may be an important reason why it has low sensitivity.

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