

Correlation between the bond dissociation energies and impact sensitivities in nitramine and polynitro benzoate molecules with polynitro alkyl groupings

Xiaoshu Song^{a,b}, Xinlu Cheng^{b,*}, Xiangdong Yang^b,
Dehua Li^c, Rongfeng Linghu^a

^a School of Physics and Chemistry, Guizhou Normal University, Guiyang 550001, China

^b Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China

^c College of Physics and Electronic Engineering, Sichuan Normal University, Chengdu 610066, China

Received 1 June 2006; received in revised form 9 November 2006; accepted 20 April 2007

Available online 4 May 2007

Abstract

The geometries of nine CHNO nitro-contained explosive molecules were fully optimized employing the B3LYP method of density functional theory with the 6-31G* basis set. The bond dissociation energy (BDE) for removal of the NO₂ group in nitroamine molecules with nitro alkyl, and benzoate with nitro alkyl were calculated at the same level. The calculational results of B3LYP/6-31G* and B3P86/6-311G* levels showed that the strength of C–NO₂ is weaker than that of N–NO₂ bond in nitroamine molecules with nitro alkyl. The weakest bond is the C–NO₂ in these computed molecules. The relationship between the impact sensitivities and the weakest C–NO₂ bond dissociation energy values was examined. The results indicate a nearly linear correlation between the impact sensitivity and the ratio of the BDE value to the molecular total energy.

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Keywords: Density functional theory; Bond dissociation energy (BDE); Nitro alkyl; Impact sensitivity; Explosives

1. Introduction

The sensitivity of an energetic material is an important parameter for indicating the stability to external stimuli such as impact, shock, and electric spark. In developing new energetic systems, one seeks optimal tradeoffs in energy content, safety, and cost. This is achieved mainly through trial. Therefore, it is desirable to try to reduce the amount of trial and error in new material development by predicting energetic material properties, including sensitivity. So, seeking the relationship between the molecular structure of energetic materials, and their sensitivities to external stimuli, have been of interest for many years [1–12]. The weakest bond breaking of the explosive molecule has been thought to be the key step in detonation initiation. Many researchers believe that C–NO₂, N–NO₂, or O–NO₂ bonds are trigger spots in nitro-contained explosives. Recently, C. J. Wu et al. stud-

ied the binary collisions of PETN and the correlation to shock sensitivity [13]. They concluded that the dissociation mechanism of PETN remains unimolecular, and the dominant reaction channel is the breaking of O–NO₂ bond. This further indicates that the strength of the weakest bond of explosive molecule plays an important role in the initiation event. The relationships between the impact sensitivities and some calculated properties of the weakest C–NO₂, N–NO₂ or O–NO₂ bond in some polynitro compounds have been widely studied [1–8]. Politzer and Murray calculated C–NO₂ and N–NO₂ bond dissociation energy in several small and moderately sized high explosives [4]. They concluded that the correlation between bond strength and impact sensitivity is not general but limited within certain classes of molecules. B.M. Rice et al. calculated C–NO₂ bond dissociation energies of some nitroaromatic molecules [5]. They concluded that there is a rough correlation between the logarithm of the impact sensitivity values $h_{50\%}$ and the BDE for rupture of the weakest bond in these molecules. Considering the complexity of detonation mechanism of high explosives, Fried et al. [12] believe that BDE is not the only factor influencing

* Corresponding author. Tel.: +86 28 85405526; fax: +86 28 85405515.

E-mail address: chengxl@scu.edu.cn (X. Cheng).

sensitivity, and the relationship involves other factors, as well. Their studies showed that the BDE scaled by energy content is a promising indicator for predicting high explosive sensitivity. In addition, Zeman's work is noticeable for its correlation between the sensitivity and the squares of detonation velocities, reciprocal temperatures and heats of fusion of the explosives, respectively [14–21]. The results of his studies on polynitro compounds showed that the relationship has different forms for different class of compounds [14–16]. His studies indicated that in those energetic materials that have similar molecular structure, the relationship between the sensitivity and the molecular structure may be easily found. Therefore, our work focuses on some high explosives, which have very similar molecular structure and similar size. In exploring the correlation with sensitivity, besides BDE, we also take into account the molecular total energy E .

We recently calculated the BDE of nitroaromatic molecules with nitro alkyl, and esters with nitro alkyl with density functional theory [22]. The results indicated a nearly linear correlation between the ratio of the bond dissociation energy to the molecular total energy (BDE/ E) and impact sensitivities in the two class energetic materials, respectively. To further substantiate the correlation and try to extend the relationship to more nitro-contained high explosives, in this work, we investigated the BDE of the other two series nitro-contained CHNO high explosives and examined the relationship between BDE/ E and impact sensitivities. The results indicate that the weakest BDE scaled by the molecular total energy indeed is a reasonable indicator for predicting high explosive sensitivity.

2. Computational methods

Geometry optimizations, energy and frequency calculations were performed for nitroamine molecules with nitro alkyl and benzoates with nitro alkyl using the Gaussian 98 package [23]. In this work, nine large size high explosive molecules (>30 atoms/molecule) were studied. Therefore, all calculations of molecular geometry and energy were performed using DFT method, Becke 3 parameters exchange and Lee, Yang and Parr correlation functionals [24,25], 6-31G* basis set, with the default Gaussian convergence criteria for the two series molecules of this work. Here, because we assume a homolytic cleavage of C–NO₂ and N–NO₂ bonds while calculating BDEs, the fragments are radical species. The calculations of

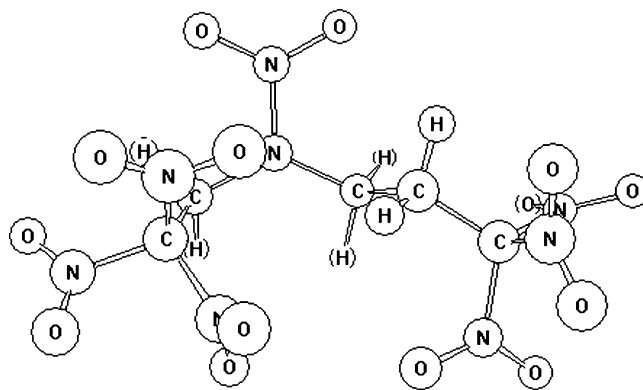


Fig. 1. The molecular structure of 2,2,2-trinitroethyl-3,3,3-trinitropropyl-nitramine.

geometry and energy for all fragments were performed using the spin-unrestricted method (UB3LYP) with the same basis set 6-31G*. The five nitroamine molecules with nitro alkyl studied are bis-(2, 2-dinitropropyl)-nitramine (C₆H₁₀N₆O₁₀), bis-(2, 2, 2-trinitroethyl)- nitramine (C₄H₄N₈O₁₄), 2,2,2-trinitroethyl-3,3,3-trinitropropyl-nitramine (C₅H₆N₈O₁₄), 2,2,2-trinitroethyl-3,3- dinitrobutyl-nitramine (C₆H₉N₇O₁₂) and trinitropropyl-(2,2-dinitropropyl)-nitramine (C₆H₉N₇O₁₂). Vibrational analyses show that the optimized structures have no imaginary frequencies. This indicates that the structure of each molecule corresponds to a local minimum on the potential energy surface. For every molecule, we optimized several possible stereoisomers, and selected the structure with the lowest energy as the most stable structure. The molecular structure of 2, 2, 2-trinitroethyl-3, 3, 3-trinitropropyl-nitramine (C₅H₆N₈O₁₄) in this class was given in Fig. 1, and the other molecules have a similar structure.

The R–NO₂ bond strength, where R denotes the remainder of the molecule, is obtained by calculating the BDE, defined here as the difference between the total energy of the parent molecule and the energies of the products of the unimolecular dissociation in which an NO₂ group is removed [5]. For example, for bis-(2, 2-dinitropropyl)- nitramine (C₆H₁₀N₆O₁₀), the BDE is:

$$\text{BDE} = [E(\text{C}_6\text{H}_{10}\text{N}_5\text{O}_8) + E(\text{NO}_2)] - E(\text{C}_6\text{H}_{10}\text{N}_6\text{O}_{10})$$

Here, the total energy of the parent molecule and the energies of the fragments were calculated using B3LYP/6-31G* and UB3LYP/6-31G* method, respectively. We calculated the BDE

Table 1
The BDEs of C–NO₂ and N–NO₂ for nitroamine explosives with nitro alkyl in different theoretical level

Explosive name	Molecular formula	BDE (kcal/mol)			
		b3lyp/6-31g*		b3p86/6-311g**	
		C–NO ₂	N–NO ₂	C–NO ₂	N–NO ₂
Bis(2,2,2-trinitroethyl)-nitramine	C ₄ H ₄ N ₈ O ₁₄	32.917	33.639	36.086	37.753
2,2,2-Trinitroethyl-3,3,3-trinitropropyl-nitramine	C ₅ H ₆ N ₈ O ₁₄	35.589	39.056	38.454	43.254
Trinitropropyl-(2,2-dinitropropyl)-nitramine	C ₆ H ₉ N ₇ O ₁₂	36.541	40.921	40.372	45.118
2,2,2-Trinitroethyl-3,3-dinitrobutyl-nitramine	C ₆ H ₉ N ₇ O ₁₂	37.175	38.432	40.488	42.635
Bis(2,2-dinitropropyl)-nitramine	C ₆ H ₁₀ N ₆ O ₁₀	36.565	39.710	40.152	41.756

NO₂ energy: –205.072206 hartrees in b3lyp/6-31G* level and –205.533512 hartrees in b3p86/6-311g** level.

of N–NO₂ and C–NO₂ for five nitroamine molecules. The results were listed in Table 1. It is clear that the C–NO₂ bond strength is weaker than the N–NO₂ bond strength. In order to make the conclusion safer, we also calculated the BDEs of N–NO₂ and C–NO₂ for five nitroamine molecules using DFT-B3P86 methods with 6-311g** basis sets. The results were also listed in Table 1. It can be seen that the results of two methods all indicate that the weakest bond is the C–NO₂ bond in the alkyl for nitroamine molecules with nitro alkyl.

3. Results and discussion

Table 2 gave the calculated strengths of the weakest bond (C–NO₂) and impact sensitivity experimental values of nitroamine explosives with nitro alkyl. The impact sensitivity values were taken from refs. [26,27].

There seems to be little apparent relationship between BDE and explosive sensitivity, but it is clear that the ratio of the bond dissociation energy to the molecular total energy (BDE/E) and the impact sensitivity have apparent correlation. Fried et al. [12] argue that BDE plays the role of an activation barrier. Once a microscopic region ignites in response to mechanical deformation, the energy released by the reaction is controlled by the energy of decomposition into equilibrium products at standard state (E_d), which is a measure of the total energy content of the material. This will in turn control the local temperature and the likelihood of a propagating chemical reaction. According to Arrhenius kinetics, the reaction velocity depends on the ratio of activation barrier to temperature. Thus Fried et al. adopt the BDE/E_d to correlate with impact sensitivity. The molecular total energy E , to some extent, reflects the E_d value in those molecules, which have similar structures. And the molecular total energy E is easily calculated with electronic structure theory. Therefore, we adopted the BDE/E to correlate with impact sensitivity $h_{50\%}$. The implication of this relationship is not very clear. But we believe that the impact sensitivity of explosives does not depend only on BDE, and the relationship involves other factors, as well. We think that the total energy E , calculated in the same theoretical level, to a great extent, represent the characteristics of the explosive molecule as a whole. The BDE/E , to some extent, should be the relative bond strength indicating the explosive stability. So, we examined the relationship between

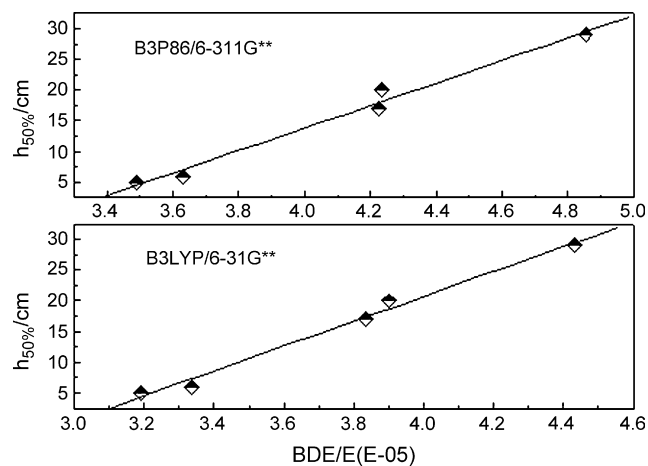


Fig. 2. Relationship between the $h_{50\%}$ and the BDE/E in nitroamine explosives with nitro alkyl in b3lyp/6-31G* and b3p86/6-311G** level.

BDE/E and impact sensitivity. Indeed, our results showed that the impact sensitivity value $h_{50\%}$ is a nearly linear function of the BDE/E. To show the relationship clearly, we gave the plot of $h_{50\%}$ versus calculated BDE/E in Fig. 2. The correlation function was given by Eq. (1). The linear correlation coefficient is 0.99.

$$h_{50\%} = -60.1806 + 20.22296 \left(\frac{BDE}{E} \right) \quad (1)$$

In order to show the generality of the linear relationship between $h_{50\%}$ and the values of BDE/E, we also calculated the BDEs using DFT-b3p86 method with 6-311g** basis sets. The results were also listed in Table 2. The plot of $h_{50\%}$ versus calculated BDE/E was also shown in Fig. 2. It can be seen that the impact sensitivity value $h_{50\%}$ still is a nearly linear function of the BDE/E in DFT-b3p86/6-311g** level. The correlation function was given by Eq. (2). The linear correlation coefficient is also 0.99.

$$h_{50\%} = -59.17809 + 18.25183 \left(\frac{BDE}{E} \right) \quad (2)$$

The second series high explosives examined here is benzoate with nitro alkyl. They are 2',2',2'-trinitroethyl-3,5-dinitrobenzoate (C₉H₅N₅O₁₂), 2',2',2'-trinitroethyl-3,5-dinitrosalicylate (C₉H₅N₅O₁₃), 2',2'-dinitropropyl-2,4,6-trinitroben-

Table 2

The molecular total energy, BDE, BDE/E and the impact sensitivities of nitroamine explosives with nitro alkyl in b3lyp/6-31G* and b3p86/6-311g** level, respectively

No.	Molecular formula	Total energy (E) (hartrees)	BDE (kcal/mol)	BDE/E (E-05)	$h_{50\%}$ ^a (cm)
1 ^b	C ₄ H ₄ N ₈ O ₁₄	-1645.154934 ^c (-1649.088762) ^d	32.917 (36.086)	3.18857 (3.4872)	5
2	C ₅ H ₆ N ₈ O ₁₄	-1684.483886 (-1688.575358)	35.589 (38.454)	3.33464 (3.6291)	6
3	C ₆ H ₉ N ₇ O ₁₂	-1519.341072 (-1523.146327)	36.541 (40.372)	3.83268 (4.2239)	17 ^e
4	C ₆ H ₉ N ₇ O ₁₂	-1519.335973 (-1523.141032)	37.175 (40.488)	3.89919 (4.2361)	20
5	C ₆ H ₁₀ N ₆ O ₁₀	-1314.869967 (-1318.231888)	36.565 (40.153)	4.43169 (4.8540)	29

^a Except when noted, experimental values were taken from ref. [25].

^b 1,2,3,4,5 represent bis (2,2,2-trinitroethyl)-nitramine, 2,2,2-trinitroethyl-3,3,3-trinitropropyl-nitramine, trinitropropyl-(2,2-dinitropropyl)-nitramine, 2,2,2-trinitroethyl-3,3-dinitrobutyl-nitramine and bis (2,2-dinitropropyl)-nitramine, respectively.

^c The values are those calculated in b3lyp/6-31g* level.

^d The values in parentheses are those calculated in b3p86/6-311g** level.

^e Experimental values were taken from ref. [26]. NO₂ energy: -205.072206 hartrees in b3lyp/6-31G* level and -205.533512 hartrees in b3p86/6-311g** level.

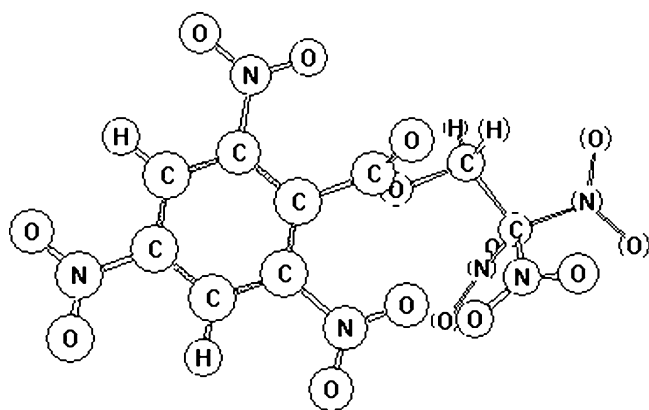


Fig. 3. The molecular structure of 2',2',2'-trinitroethyl-2,4,6-trinitrobenzoate.

zoate ($C_{10}H_7N_5O_{12}$) and 2',2',2'-trinitroethyl-2,4,6-trinitrobenzoate ($C_9H_4N_6O_{14}$), respectively. We also gave the structure of one molecule of this class in Fig. 3. It is clear that the H atom of the carboxyl is replaced by an alkyl in every molecule of this class and two or three H atoms of the alkyl are replaced by NO_2 .

The computed results indicated that there is also a nearly linear correlation between the ratio of the bond dissociation energy to the molecular total energy (BDE/E) and the impact sensitivity in this series explosive. And it is very similar in the case of the nitroamine molecules with nitro alkyl.

Table 3 gave the calculated (B3LYP/6-31G* level) strengths of the weakest bond (C– NO_2) and impact sensitivity experimental values of these molecules. The impact sensitivity values were taken from ref. [28]. The plot of $h_{50\%}$ versus calculated BDE/E was given in Fig. 4. The function relationship was given by Eq. (3). The linear correlation coefficient is 0.99.

$$h_{50\%} = -524.83252 + 154.26028 \left(\frac{BDE}{E} \right) \quad (3)$$

Generally, while calculating BDE values, zero point vibrational energy (ZPVE) corrected energies had to be used and basis set superposition error (BSSE) calculations had to be performed. Here, we are mainly concerned with the relationship between the BDE/E and $h_{50\%}$. It is reasonable to assume that the ZPVE and BSSE corrected energies have little influence on the relationship of molecules, which have similar structure. However, in order to test this assumption, we examined the BDE and BDE/E in which the ZPVE and BSSE are under consideration. The results

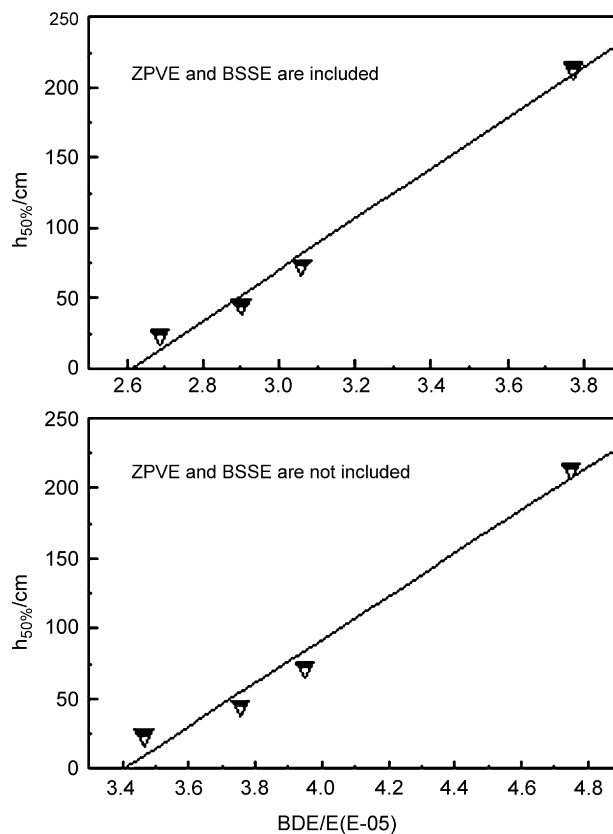


Fig. 4. Relationship between the $h_{50\%}$ and the BDE/E in benzoates with nitro alkyl when ZPVE and BSSE are and are not included.

were also listed in Table 3. The plot of $h_{50\%}$ versus calculated BDE/E was also given in Fig. 4. The function relationship was given by Eq. (4). The linear correlation coefficient is 0.99.

$$h_{50\%} = -472.07685 + 180.72844 \left(\frac{BDE}{E} \right) \quad (4)$$

We can see that the impact sensitivity value $h_{50\%}$ is still a nearly linear function of the BDE/E when the ZPVE and BSSE corrections are taken into account. Namely, the ZPVE and BSSE corrections have little influence on the linear relationship. Therefore, the ZPVE and BSSE corrections have not been considered in the calculation of BDE and BDE/E for five nitroamine molecules with nitro alkyl.

It is obvious that the result of this work is completely in agreement with that of our previous work [22]. This further substantiated the correlation between the BDE/E and the sen-

Table 3

The total energy, BDE, BDE/E and the impact sensitivities of benzoates with nitro alkyl when ZPVE and BSSE are and are not included, respectively

Explosive name	Molecular formula	Total energy (E) (hartrees)	BDE (kcal/mol)	BDE/E (E-05)	$h_{50\%}$ ^a (cm)
2',2',2'-Trinitroethyl-3,5-dinitrobenzoate	$C_9H_5N_5O_{12}$	-1521.876544 (-1521.693213)	37.699 ^b (29.209) ^c	3.948 (3.059)	73
2',2',2'-Trinitroethyl-3,5-dinitrosalicylate	$C_9H_5N_5O_{13}$	-1597.096494 (-1596.908340)	37.642 (29.111)	3.756 (2.905)	45
2',2',2'-Trinitroethyl-2,4,6-trinitrobenzoate	$C_9H_4N_6O_{14}$	-1726.348222 (-1726.163314)	37.536 (29.088)	3.465 (2.685)	24
2',2'-Dinitropropyl-2,4,6-trinitrobenzoate	$C_{10}H_7N_5O_{12}$	-1561.205160 (-1560.993259)	46.518 (36.965)	4.748 (3.774)	214

^a Experimental values were taken from ref. [27].

^b The values are those in which the ZPVE and BSSE are not included.

^c The values in parentheses are those in which the ZPVE and BSSE are included.

sitivity in those energetic materials that have similar molecular structure.

4. Conclusion

The BDE for removal of the NO₂ group in nitroamine molecules with nitro alkyl, and benzoates with nitro alkyl were calculated using DFT-B3LYP/6-31G* and DFT-B3P86/6-311G** methods. The results further substantiated the correlation between the weakest BDE and the explosive sensitivity. It is found that the ratio of the weakest BDE to the molecular total energy has a nearly linear correlation with the impact sensitivity values $h_{50\%}$. This indicates that the BDE/*E* is a reasonable practical indicator of explosive sensitivity. Since this indicator is easily computed with electronic structures, it may prove useful in the design of new energetic materials.

Acknowledgements

This project was supported by the National Natural Science Foundation of China and CAEP under grant No. 10676025 and No. 10376021, by the Research Fund for the Doctoral Program of High Education of China under grant No. 20050610010, and by the Research Foundation of Education Bureau of Guizhou Province of China under grant No. 2006204.

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