ARTICLE

Quantum Chemical Studies on Structure and Detonation Performance of Bis(2,2-dinitropropyl ethylene)formal

Shu-qing Yan[a], Xiao-hong Li[b]*

a. School of Mathematics and Information Science, North China University of Water Resources and Electric Power, Zhengzhou 450011, China
b. College of Physics and Engineering, Henan University of Science and Technology, Luoyang 471003, China

Based on the full optimized molecular geometric structures via B3LYP/6-311+G(2d,p) method, a new gem-dinitro energetic plasticizer, bis(2,2-dinitropropyl ethylene)formal was investigated in order to search for high-performance energetic material. IR spectrum, heat of formation, and detonation performances were predicted. The bond dissociation energies and bond orders for the weakest bonds were analyzed to investigate the thermal stability of the title compound. The results show that the four N-NO$_2$ BDEs are nearly equal to the values of 164.38 kJ/mol, which shows that the title compound is a stable compound. The detonation velocity and pressure were evaluated by using Kamlet-Jacobs equations based on the theoretical density and condensed HOF. The crystal structure obtained by molecular mechanics belongs to P2$_1$ space group, with lattice parameters Z=2, a=13.8017 Å, b=13.4072 Å, c=5.5635 Å.

Key words: Density functional theory, Detonation property, Thermal stability, bis(2,2-dinitropropyl ethylene) formal

I. INTRODUCTION

The demand for high-performance explosives and propellants has led to intensive investigations on improving their energetic, mechanical, and storage properties and safe handling. Attempts have focused primarily on using more energetic ingredients like binders, plasticizers, *etc.* It has been reported that plasticizers in combination with a binder aid in processing of propellants by achieving optimum viscosity [1] and the molecular structure and quantity available in the plasticizer system significantly affect the mechanical properties of the propellant [2, 3]. In modern energetic propellant composition, conventional plasticizers are being gradually replaced by energetic plasticizers which have azido, nitro ester, fluoronitro, fluoroamino, nitro groups or combination of energetic groups in the same molecule [4−9]. Of these, nitrate ester groups are a fertile source of energetic plasticizers. Some energetic plasticizers containing nitrate ester groups are synthesized [10−13].

Energetic plasticizers containing the gem-dinitro groups have generally low sensitivity to unplanned stimuli and are attractive due to their high oxygen content and high energy. These gem-dinitro energetic

plasticizers are frequently prepared by a reaction of nitro alcohols and formaldehyde in the presence of an acid [14−19], including bis(2,2-dinitropropyl)acetal (BDNPA), bis(2,2-dinitrobutyl)formal (BDNBF), and bis(2,2-dinitropropyl)diformal (BDNPDF).

Optimum energetic plasticizers need to have low viscosity, low sensitivity to stimuli, high thermal stability, and high oxygen balance [20]. But these demands are contradictory and no existing energetic plasticizers can achieve the ideal requirements, despite the large number of energetic plasticizers developed so far. In view of this, a new gem-dinitro energetic plasticizer, bis(2,2-dinitropropyl ethylene)formal (BDNPEF), has been studied in detail due to the good compatibility with polyether-based polyurethane binders.

The cost and danger associated with synthesizing and testing new energetic plasticizers have driven to computationally assist the design of energetic plasticizers. Theoretical studies not only make it possible to screen candidate compounds, but also provide understanding in terms of the relationships between molecular structure and properties [21, 22].

In the present study, density functional theory and molecular mechanics (MM) methods were employed to evaluate crystal structure and properties of BDNPEF, such as heat of formation, infrared spectrum, thermodynamic properties, detonation performance and thermal stability. The molecular structure is shown in Fig.1. The calculation results show that BDNPEF may be a

---

*Author to whom correspondence should be addressed. E-mail: Lorna639@163.com
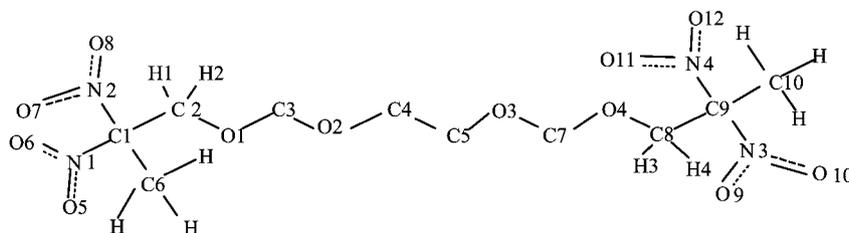
FIG. 1 Molecular framework of BDNPEF.

very promising high-energy plasticizer.

II. METHODS AND COMPUTATIONAL DETAILS

Computations were performed with Gaussian 03 package [23] at B3LYP [24−26] method with 6-311+G(2d,p) basis set. The geometric parameters were allowed to be optimized and no constraints were imposed on molecular structure during optimization process. Vibrational analysis was performed thereafter at the same level with the Gaussian 03 program package. The optimized structure was characterized to be true local energy minima on potential energy surfaces without imaginary frequencies. On the basis of the principle of statistical thermodynamics [27], standard molar heat capacity ($C_{p,m}^0$), standard molar entropy ($S_{p,m}^0$), and standard molar enthalpy ($H_{p,m}^0$) from 200 K to 800 K were derived from the scaled frequencies using a self-compiled program.

The natural bond orbital (NBO) calculations were performed using the NBO 3.1 program as implemented in the Gaussian 03 package at B3LYP/6-311+G(2d,p) level in order to understand various second-order interactions between the filled orbitals of one subsystem and vacant orbitals of another subsystem, which is a measure of the intermolecular delocalization or hyperconjugation.

To measure the strength of bonds and relative stability of the molecule, the bond dissociation energies (BDEs) of various bonds in molecule are calculated. BDE is the required energy in homolysis of a bond and is commonly denoted by difference between total energies of product and reactant after zero point energy correction. The expressions for the homolysis of $R_1−R_2$ bond and calculation of BDE are shown as follows:

$$R_1 - R_2(g) \rightarrow R_1 \cdot (g) + R_2 \cdot (g) \tag{1}$$
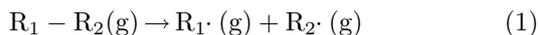
$$\begin{aligned} BDE(R_1 - R_2) = H_{298}(R_1 \cdot) + H_{298}(R_2 \cdot) - \\ H_{298}(R_1 - R_2) \end{aligned} \tag{2}$$

where $R_1−R_2$ denotes the neutral molecule, and $R_1 \cdot$ and $R_2 \cdot$ stand for the corresponding product radicals after the bond dissociation, $BDE(R_1−R_2)$ is the bond dissociation enthalpy of the bond $R_1−R_2$. The latter three items in Eq.(2) are the enthalpies of the corresponding radicals and the parent compound, respectively.

Detonation velocity (D) and pressure (P) are the most important targets of scaling the detonation characteristics of energetic materials. For the explosives with C, H, N and O elements, these parameters can be calculated using the Kamlet-Jacbos (K-J) equations [28]:

$$D = 1.01\Phi^{0.5}(1.0 + 1.3\rho) \tag{3}$$

$$\Phi = N\bar{M}^{0.5}Q^{0.5} \tag{4}$$

$$P = 1.558\Phi\rho^2 \tag{5}$$

where ρ is the packed density, N is the moles of gas produced by per gram of explosives, $\bar{M}$ is an average molar weight of detonation products, and Q is the estimated heat of detonation. N, $\bar{M}$, and Q are determined according to the largest exothermic principle [29].

Since the condensed phase for most energetic compounds is solid, the calculation of detonation properties requires solid phase heat of formation (HOF) ($\Delta H_{f,solid}$). According to Hess's law of constant heat summation [30], the gas-phase HOF ($\Delta H_{f,gas}$) and heat of sublimation ($\Delta H_{f,sub}$) can be used to evaluate the solid phase HOF:

$$\Delta H_{f,solid} = \Delta H_{f,gas} - \Delta H_{f,sub} \tag{6}$$

Politzer *et al.* found that the heats of sublimation can correlate well with the molecular surface area and electrostatic interaction index $\nu\delta_{tot}^2$ of energetic compounds [31, 32]. The empirical expression of the approach is as follows:

$$\Delta H_{sub} = aA^2 + b\sqrt{\nu\delta_{tot}^2} + c \tag{7}$$

where A is the surface area of the 0.001 electron/bohr^3 isosurface of electronic density of the molecule, ν describes the degree of balance between positive and negative potential on the isosurface, and δ_{tot}^2 is a measure of variability of the electrostatic potential on the molecular surface. The coefficients a, b, and c were determined by Rice and coworker [33]: a=2.670×10^{-4} kcal/mol, b=1.650 kcal/mol and c=2.966 kcal/mol. The descriptors A, ν and δ_{tot}^2 were calculated using the computational procedures proposed by Lu [34].

The possible polymorphs and crystal structure of the title compound were predicted by rigorous molecular packing calculations using polymorph module of Material Studio [35] since high-energy compounds are usually

TABLE I Selected bond lengths and angles of the title compound computed at B3LYP/6-311+G(2d,p) level.

Bond length/Å		Bond angle/(°)	
N1−C1	1.535	N1−C1−N2	104.25
C1−N2	1.524	N1−C1−C6	107.67
C1−C6	1.504	C6−C1−C2	109.67
C1−C2	1.518	C1−C2−O1	106.15
C2−O1	1.411	C2−O1−C3	113.50
O1−C3	1.385	O1−C3−O2	109.22
C3−O2	1.402	C3−O2−C4	112.29
O2−C4	1.411	O2−C4−C5	107.39
C4−C5	1.510	C4−C5−O3	107.08

in condensed phases, especially solid form. The compass force-field is used to search the possible molecular packing among the most probable seven space groups (P2$_1$/c, P-1, P2$_1$2$_1$2$_1$, Pbca, C2/c, P2$_1$, and Pna2$_1$) [36, 37].

III. RESULTS AND DISCUSSION

A. Optimized structures

It is necessary to study the geometric structures before discussing other properties. Some bond lengths and angles obtained from B3LYP/6-311+G(2d,p) method are tabulated in Table I. From Table I, it is noted that the C−N bond lengths range from 1.524 Å to 1.535 Å, which are longer than the normal C−N single bond length (1.47 Å) [38]. The C−O bond lengths of BDNPEF range from 1.380 Å to 1.415 Å, which are shorter than that of the usual C−O (1.42 Å). These varieties of C−O bond lengths are mainly due to the electronic delocalization in molecule.

B. Infrared spectra

The IR spectrum is one basic property of a compound and often used to analyze or identify substances. Therefore, it is of great significance to calculate the IR spectrum of the title compound by a theoretical method. Here, vibrational frequencies were calculated by using DFT B3LYP/6-311+G(2d,p) level. Figure 2 presents the simulated IR spectrum based on the scaled harmonic vibrational frequencies for BDNPEF.

For BDNPEF, there are five main characteristic regions. The modes in 2900−3188 cm^{-1} are associated with C−H stretch. In this region, the strongest characteristic peak is at 3052 cm^{-1}. The modes in 1620−1708 cm^{-1} are associated with the N=O asymmetric stretch of nitro groups and the strong characteristic peak is at 1660 cm^{-1}. The modes in 1340−1492 cm^{-1} are associated with the C−H bend-
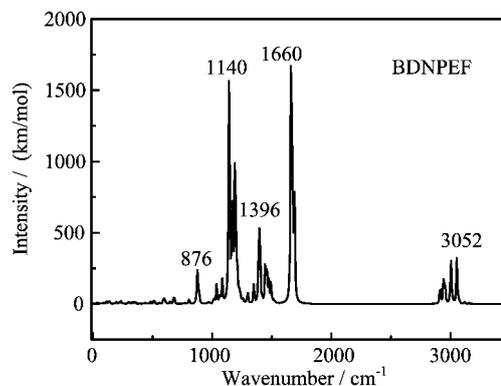

FIG. 2 The simulated infrared spectrum for BDNPEF.

TABLE II Calculated energies and HOF of species.

Compound	E_0/a.u.	HOF/(kJ/mol)
CH$_4$	−40.670367	−74.4 [40]
CH$_3$NO$_2$	−245.614467	−80.8 [40]
C$_2$H$_6$	−80.109865	−84.6 [40]
CH$_3$OCH$_3$	−155.466334	−184.1 [41]
BDNPEF	−1516.898265	−774.0

ing. The modes in 1037−1228 cm^{-1} are mainly associated with C−O stretch together with the C−H bending, and the strongest characteristic peak is at 1140 cm^{-1}, which corresponds to the C−O stretch. The modes below 1000 cm^{-1} are associated with the C−N stretch, the rocking of nitro groups and methyl groups together with the CNO bending.

C. Heat of formation

HOF is an important parameter for calculation of the detonation performance and can be used to estimate the amount of energy released or absorbed in a chemical reaction. Increasing the HOF will generally increase the detonation performance. One can obtain the standard HOF at 298.15 K through using the atomization reaction or isodesmic reaction method. In this work isodesmic reaction method was employed [39].

The accuracy of HOF obtained theoretically was conditioned by the reliability of HOF of the reference compounds. The HOF for BDNPEF can be derived from the isodesmic reaction, shown in Fig.3.

Table II lists the total energies (E_0), $\Delta H_{\mathrm{f,gas}}$ of the reference compounds involved in the reaction. The calculated HOF for BDNPEF is also included.

D. Detonation properties

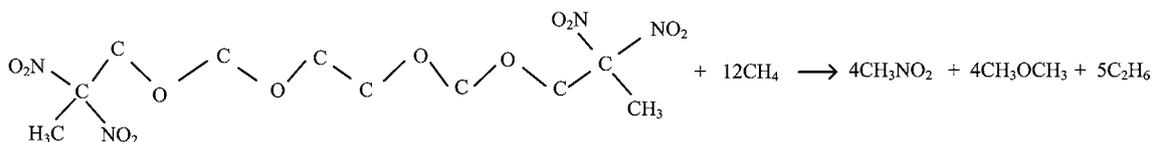Detonation velocity D and pressure P are the important parameters to evaluate the performances of en-

FIG. 3 The isodesmic reaction.

TABLE III Predicted density and detonation properties of the title compound.

Property	BDNPEF	TNT [42]
A	397.1961	
ν	0.24436764	
$\nu\delta_{\text{tot}}^2$	29.56319	
$\Delta H_{\text{f,sub}}$/(kJ/mol)	17.3	
$\Delta H_{\text{f,solid}}$/(kJ/mol)	−791.3	
V/(cm^3/mol)	249.034	
ρ/(g/cm^3)	1.55	1.65
D/(km/s)	7.08	7.02
P/GPa	20.20	20.7

ergetic materials. As for C, H, O, and N-containing explosives, they can be estimated using the K-J equations [28]. In this work, we computed the condensed phase heat of formation of the title compound through the method of Byrd and Rice [33].

Density is one of the critical factors that determine the energetic properties of compounds. According to the K-J equations [28], density greatly affects the detonation performance. Detonation pressure is dependent on the square of the density, while detonation velocity is proportional to the density. In the work, we calculated the density of the title compounds using the method of Politzer [31]. In addition, it is noted that detonation pressure and velocity are overestimated if gas phase HOFs instead of solid phase values are used [30]. Using Eqs. (5), (6) and the computational procedures proposed by Lu [34], the $\Delta H_{\text{f,solid}}$, $\Delta H_{\text{f,sub}}$ and the related descriptors A, ν and δ_{tot}^2 are obtained.

Table III lists the surface area A, ν, δ_{tot}^2, $\Delta H_{\text{f,sub}}$, $\Delta H_{\text{f,solid}}$, V, ρ, D, and P of the title compound. In order to have a comparison, the ρ, D, and P of trinitrotoluene (TNT) are also included [42].

Obviously, the detonation velocity and pressure of BDNPEF (D=7.08 km/s, P=20.20 GPa) are comparable to TNT. This shows that BDNPEF is a potential energetic material.

E. Thermal stability

For the energetic materials, it is of practical interest whether they are thermodynamically stable enough. A good energetic material should have a high stability. Thus, studies on the bond dissociation or pyrolysis

mechanism are important to understand the decomposition process of the energetic materials because they are directly relevant to the sensitivity and stability of the energetic compounds. For some compounds, a key initiating step appears to be the rupture of a particular bond, a "trigger linkage" [31]. At present, there is a consensus that nitro groups often represent the primary cause of initiation reactivity of organic polynitro compounds [43−45].

In this work, two possible initial steps, *i.e.* the breakings of C1−N1 and C1−N2 bonds (or C9−N3 and C9−N4 bonds) for BDNPEF in the chain, are considered. The calculated results show that the C1−N1 and C1−N2 BDEs are nearly equal and are all 164.38 kJ/mol. Obviously, the title compound is a stable compound according to the stability request of HEDC (BDE≈80−120 kJ/mol).

F. Molecular packing prediction and density

The crystal structure of the title compound in this work is predicted by COMPASS force field [46], which can produce the gas- and condensed-phase properties reliably for a broad range of systems [47]. Using COMPASS force field, we can pack arrangements in all reasonable space groups to search for the low-lying minima in the lattice energy surface. The structure optimized by B3LYP/6-311+G(2d,p) method is considered as input structure for polymorph search. Table IV lists the lattice parameters in all reasonable space groups.

It is noted from Table IV that the energies range from −47.9 to −65.1 kJ/(mol·cell) and the structure with P2$_1$ symmetry has the lowest energy. Most stable polymorph usually possesses the least energy at 0 K, so the title compound tends to exist in the P2$_1$ group. The corresponding lattice parameters are Z=2, a=13.8017 Å, b=13.4072 Å, c=5.5635 Å, ρ=1.60 g/cm^3. Figure 4 gives the molecular packing of the title compound in P2$_1$ space group.

G. Thermodynamic properties

Based on the scaled vibrational frequencies, the thermodynamic functions including standard molar heat capacity $C_{\text{p,m}}^0$, entropy $S_{\text{p,m}}^0$ and enthalpy $H_{\text{p,m}}^0$, are obtained based on statistical thermodynamic principle. The temperature-dependent relations for the thermody-

TABLE IV Unit cell parameters of the possible molecular packings of the title compound.

Space group	Z	E/(kJ/mol cell)	ρ/(g/cm^3)	a/Å	b/Å	c/Å	α/(°)	β/(°)	γ/(°)
C2/c	8	−49.3	0.65	25.7135	16.4954	11.3111	90.00	110.80	90.00
P1	2	−47.9	0.07	14.9854	6.0009	14.1641	81.24	70.16	41.39
P2$_1$2$_1$2$_1$	4	−62.6	1.46	14.8012	6.3959	16.9540	90.00	90.00	90.00
P2$_1$	2	−65.1	1.60	13.8017	13.4072	5.5635	90.00	48.90	90.00
P2$_1$/c	4	−63.9	1.50	5.5040	19.1759	18.2954	90.00	116.93	90.00
Pna2$_1$	4	−62.7	1.55	17.0191	17.6230	5.4186	90.00	90.00	90.00
Pbca	8	−61.1	0.51	16.4296	8.4139	22.7930	90.00	90.00	90.00
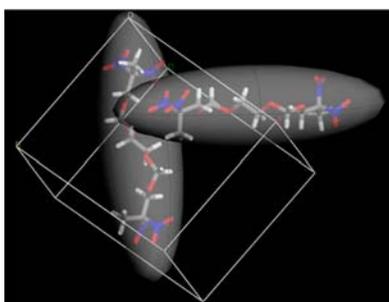
FIG. 4 Molecular packing of the title compound in P2$_1$ space group.
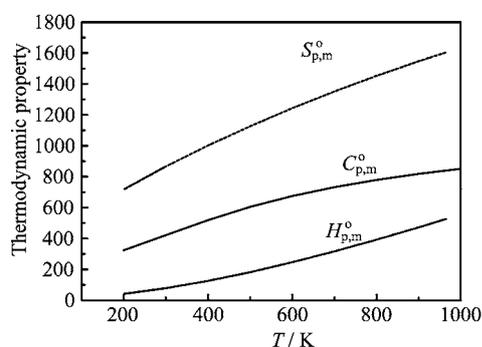
FIG. 5 The relationships between the thermodynamic functions and temperature T for the title compound.

namic functions are as follows and expressed in Fig.5.

$$C_{p,m}^0 = 157.30 + 1.01T - 3.14 \times 10^{-4}T^2 \qquad (8)$$

$$S_{p,m}^0 = 452.12 + 1.47T - 2.91 \times 10^{-4}T^2 \qquad (9)$$

$$H_{p,m}^0 = -74.57 + 0.45T + 1.81 \times 10^{-4}T^2 \qquad (10)$$

The corresponding correlation coefficients for $C_{p,m}^0$, $S_{p,m}^0$, and $H_{p,m}^0$ are 0.9935, 0.9996, and 0.9994. It is noted that all thermodynamic properties increase with the increase of temperature because of the larger contribution of vibrational movement at the higher temperature.

IV. CONCLUSION

In this work, a new gem-dinitro energetic plasticizer, bis(2,2-dinitropropyl ethylene) formal was investigated theoretically by using B3LYP/6-311+G(2d,p) method. Compared with TNT, the title compound is a potential energetic material with the predicted detonation velocity (7.08 km/s) and detonation pressure (20.20 GPa). Based on the results of bond order and bond dissociation energy, the four N−NO$_2$ BDEs are nearly equal and are all 164.38 kJ/mol, which shows that the title compound is a stable compound. In addition, the most possible space group of the title compound predicted by COMPASS force field is P2$_1$ space group.

V. ACKNOWLEDGMENTS

[1] A. Provatas, *Energetic Polymers and Plasticizers for Explosive Formulations-A Review of Recent Advances*, DSTO-TR-0966, (2000).

[2] X. H. Li, Z. X. Tang, X. Z. Zhang, and X. D. Yang, J. Hazard. Mater. **165**, 372 (2009).

[3] A. Provatas, *Characterization and Polymerization Studies of Energetic Binder Systems*, DSTO-TR-1171, (2001).

[4] J. P. Agrawal and R. D. Hodgson, *Organic Chemistry of Explosives*, West Sus sex, England: John Wiley & Sons Ltd., (2007).

[5] J. X. Shao, X. L Cheng, and X. D Yang, Chin. Phys. **15**, 329 (2006).

[6] Y. P. Ji, P. R. Li, W. Wang, Y. Lan, and F. Ding, Chin. J. Explos. Propellants **28**, 47 (2005).

[7] J. X. Shao, X. L Cheng, and X. D. Yang, Struct. Chem. **16**, 457 (2005).

[8] R. H. Taylor and H. Ala, US Patent 5579634, (1996).

[9] K. Menke and S. Eisele, Propellants Explos. Pyrotech. **22**, 112 (1997).

[10] N. Marsh and A. Marsh, Clin. Exp. Pharmacol. Physiol. **27**, 313 (2000).

[11] J. Akhavan, *The Chemistry of Explosives*, 2nd Edn, UK: The Royal Society of Chemistry, (2004).

[12] A. T. Camp, L. A. Dickinson, and P. R. Mosher, US Patent 3634158, (1972).

[13] S. B. Preston, US Patent 5454891 (1995).

[14] M. A. Barrio, J. Hu, P. Z. Zhou, and N. Cauchon, J. Pharm. Biomed. Anal. **41**, 738 (2006).

[15] M. Jang and R. M. Kamens, Environ. Sci. Technol. **35**, 4758 (2001).

[16] J. S. Kim, J. R. Cho, K. D. Lee, and J. K. Kim, US Patent 0056663 (2007).

[17] M. A. Lenskii, E. E. Shul'ts, A. A. Androshchuk, and G. A. Tolstikov, Russ. J. Org. Chem. **45**, 1772 (2009).

[18] K. C. Barsanti and J. F. Pankow, Atmos. Environ. **38**, 4371 (2004).

[19] M. Jang, N. M. Czoschke, S. Lee, and R. M. Kamens, Science **298**, 814 (2002).

[20] Y. Chen, Y. Kwon, and J. S. Kim, J. Ind. Eng. Chem. **18**, 1069 (2012).

[21] X. H. Li, Z. M. Fu, and X. Z. Zhang, Struct. Chem. **23**, 515 (2012).

[22] X. H. Li, R. Z. Zhang, and X. Z. Zhang, Struct. Chem. **24**, 393 (2013).

[23] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W.Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, *Gaussian 03, Revision B.02*, Pittsburgh PA: Gaussian Inc., (2003).

[24] A. D. Becke, J. Chem. Phys. **97**, 9173 (1992).

[25] C. Lee, W. Yang, and R. G. Parr, Phys. Rev. B **37**, 785 (1988).

[26] A. D. Becke, J. Chem. Phys. **98**, 5648 (1993).

[27] T. L. Hill, *Introduction to Statistic Thermodynamics*, New York: Addison-Wesley, (1960).

[28] M. J. Kamlet and S. J. Jacobs, J. Chem. Phys. **48**, 23(1968).

[29] X. H. Zhang and Z. H. Yun, *Explosive Chemistry*, Beijing: National Defence Industry Press, (1989).

[30] P. W. Atkins, *Physical Chemistry*, Oxford: Oxford University Press, (1982).

[31] P. Politzer, P. Lane, and J. S. Murray, Cent. Eur. J. Energ Mater. **8**, 39(2011).

[32] P. Politzer and J. S. Murray, Cent. Eur. J. Energ. Mater. **8**, 209 (2011).

[33] E. F. C. Byrd and B. M. Rice, J. Phys. Chem. A **110**, 1005 (2006).

[34] T. Lu, *Multiwfn Revision 2.5.2*, Beijing: Beijing Science and Technology, (2012).

[35] *Materials Studio Blends Module, Version 4.4, Software for Miscibility Estimation: Theory in Blends*, San Diego, CA: Accelrys Software Inc., (2008).

[36] A. D. Mighell, V. L. Himes, and J. R. Rodgers, Acta Crystallogr. **39**, 737 (1983).

[37] R. Srinivasan, Acta Crystallogr. A **48**, 917 (1992).

[38] Y. Sasada, *Molecular and Crystal Structures in Chemistry Handbook, 3rd Edn.* Maruzen, Tokyo: The Chemical Society of Japan, (1984).

[39] W. J. Hehre, L. Radom, and P. V. R. Schleyer, *Ab initio Molecular Orbital Theory*, New York: Wiley, (1986).

[40] D. R. Lide, *Handbook of Chemistry and Physics,* 84th Edn., Boca Raton, FL: CRC Press LLC, (2004).

[41] G. Pilcher, A. S. Pell, and D. J. Coleman, Trans. Faraday Soc. **60**, 499 (1964).

[42] H. M. Xiao, *Structures and Properties of Energetic Compounds*, Beijing: National Defense Industrial Press, (2004).

[43] X. H. Li, R. Z. Zhang, and X. Z. Zhang, Struct. Chem. **22**, 577 (2011).

[44] X. H. Li, R. Z. Zhang, X. D. Yang, and H. Zhang, J. Mol. Struc.: THEOCHEM **815**, 151 (2007).

[45] X. H. Li, R. Z. Zhang, and X. Z. Zhang, J. Hazard. Mater. **183**, 622 (2010).

[46] H. Sun, J. Phys. Chem. B **102**, 7338 (1998).

[47] X. J. Xu, W. H. Zhu, and H. M. Xiao, J. Phys. Chem. B **111**, 2090 (2007).