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SIMPLE WAY TO PREDICT ELECTROSTATIC SENSITIVITY OF NITROAROMATIC COMPOUNDS

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Abstract. In this paper, a new simple method is introduced to predict electrostatic sensitivity of nitroaromatic compounds. This technique uses the calculated detonation velocity at maximum nominal density and the contribution of some structural parameters. A training set is used to optimize the new correlation. The predicted results for 17 explosives are also compared with quantum mechanical computations, for some explosives in which deviations of quantum mechanical calculations from experimental data are low. The root mean square deviations (rms) from experiment for introduced model and complicated quantum mechanical computation are the same, i.e. 2.0 J.

Keywords: electrostatic sensitivity, nitroaromatic, detonation velocity, correlation

1. Introduction

Predicting various properties of new energetic compounds before the expenditure connected with their development and synthesis is very important to chemist and chemical industries. The search for new explosives is most concerned with detonation performance, thermal properties and sensitivity. Theoretical methods can help the chemists to develop systematic and scientific formulations of appropriate futuristic target molecules having complementary properties of good thermal stability, sensitivity and enhanced explosive performance. The major goal of these methods is to pro-

vide reliable predictive tools and understanding the molecules which are responsible for desired properties. As representative example, some various empirical methods have been recently introduced to predict detonation velocity of ideal and non-ideal explosives through different models [1-7].

Stimuli can cause detonation which may be included impact, shock, electric spark, heat and friction. However, different kinds of sensitivity have been identified in terms of stimuli causing detonation. The electric spark or electrostatic sensitivity (E_{ES}) of an energetic compound is an important quantity which can be defined as the degree of sensitivity to the electrostatic discharge. It can be predicted by the electrostatic discharge energy required for 50% initiation probability. Measurements of E_{ES} can be carried out with the help of the apparatus and procedures which were described elsewhere [8]. Zeman and coworkers [9-12] have found that there are some correlations for special groups of energetic compounds among detonation velocity, the Piloyan activation energy of decomposition from the differential thermal analysis (DTA) and electrostatic spark sensitivity. They have also indicated that there was a linear relationship between the electrostatic spark energy values and the squares of detonation velocities for some special groups of explosives. Later, Wang et al. [13,14] have used quantum chemistry methods to optimize molecular geometries and electronic structures for some explosives. They have computed crystalline density and heat of formation to predict detonation pressure through Kamlet and Jacobs correlation [15]. However, they have indicated that there were quantitative relationships between the experimental electrostatic spark sensitivity values and predicted values of detonation velocity and pressure for some special groups of energetic compounds. The purpose of this work is to predict a general new correlation between electrostatic sensitivity and detonation velocity at maximum nominal density as well as molecular structure of nitro arene energetic compounds. To predict detonation velocity at maximum nominal density, a new method has been used for this purpose [16]. This work shows how a reasonable good correlation can be obtained between electrostatic sensitivity and calculated detonation velocity at maximum nominal density as well as some structural parameters. One set of explosives is used as training set to establish a new correlation. The predicted results for the second set, as test set, are compared to computed results of quantum mechanical method [13].

2. Sensitivity

Sensitivity for energetic materials is a complex problem. Impact sensitivity is the most commonly used to show sensitivity. Reliable experimental results for impact test are known to be relatively difficult because difficulty associated with puzzles in initiation mechanism of explosion caused by mechanical impacts. The results of impact sensitivity are often not reproducible because factors in the impact experiment that might affect the formation and growth of hot spots could strongly affect the measure-

ments. Thus, data of impact sensitivities are extremely sensitive to the conditions under which the tests can be performed. The impact sensitivity has been the most intensively studied despite large errors present in some of experimental data [17].

Shock sensitivity is another convenient kind of sensitivity. It can be measured by a standard small or large scale gap test [18] and is interpreted as being directly proportional to the maximum gap width through which a given shock wave generated by another explosive such as RDX. Reliable shock sensitivity tests exist but there are the same questions about the mechanisms of initiation for both the impact and shock tests. Some studies have been performed to establish some correlations between shock sensitivity and computed results of quantum mechanical methods or structural parameters [18-22].

Since there is no unique idea of initiation mechanism of energetic materials by electrostatic spark [9], the primary fragmentation reactions in this initiation can be supposed identical with the primary splitting processes of low-temperature thermolysis and detonation transformation of molecules of these materials [10]. The mechanism of energy transfer from electrostatic spark to the reaction center of molecule is not fully understood yet [9,10] so that some authors were inclined to the idea of conversion of the electrostatic spark energy into a thermal effect, i.e. to a thermolytic principle of the electrostatic spark initiation [23,24]. The initiation can be considered as a multidisciplinary problem because mechanism of the spark energy transfer can be related to molecular structure, thermal reactivity, sensitivity to mechanic stimuli and parameters of their detonation [9-11,23-25].

3. Detonation at maximum nominal density

Detonation velocity at maximum nominal or theoretical density is very important in armament design because it introduces the explosives with higher density which is preferred for warheads used in missiles and ammunitions. It was recently shown that detonation velocity at maximum nominal density can correlate with the explosive's elemental composition and some structural parameters. The new method can give reliable results for any pure or mixed $C_aH_bN_cO_d$ explosives [16]. It is also of significant value because maximum initial density and the heat of formation are rarely known experimentally. For the new explosive of interest, detonation velocity at maximum nominal density can be expressed as follows:

$$D_{\max} = 7.68 - 0.198a - 0.111b + 0.294c + 0.0742d - 0.635n_{NR} - 0.735n_{mN} \quad (1)$$

where $D_{\max}$ is detonation velocity at maximum nominal density in km/s, n_{NR} is the number of $-N=N-$ or NH_4^+ in explosive and n_{mN} is the number of nitro groups ($-NO_2$) attached to carbon in nitrocompounds in which $a = 1$.

4. Results and discussion

4.1. Correlation between E_{ES} and D_{max}

The study of electrostatic spark sensitivity of nitro arene compound has indicated that the measured electrostatic spark sensitivity can correlate with detonation velocity at maximum nominal density and some structural parameters. As seen in previous section, it is possible to predict detonation velocity via elemental composition and some specific structural parameters [16] rather than using complicated quantum chemistry computer programs [13,14]. It was found that the existence of some specific groups such as hydroxyl ($-OH$) group and the number of amino ($-NH_2$) group can affect the values of electrostatic spark sensitivity [13]. However, the study has shown that the following general equation based on multiple linear regression method can be used to find electrostatic spark sensitivity:

$$E_{ES} = w_1 + w_2 D_{max} + w_3 C_{SG} + w_4 n_{-NH_2, -HNCO-} \quad (2)$$

where w_1 to w_4 are adjustable parameters which can be obtained by the best fit to experimental electrostatic sensitivities data via multiple linear regression method [26], C_{SG} is the presence of special groups and $n_{-NH_2, -HNCO-}$ is the number of $-NH_2$ or $-HNCO-$ groups attached to aromatic ring. Wang and coworkers [13,14] have found that the energetic compounds with some specific groups have different electrostatic sensitivity. Although they considered large sets of different groups, it was found the contribution of $-OH$, $-N=N-$, $-OR$ and $-S(O_2)-$ are important in predicting electrostatic spark sensitivity [27]. Moreover, it can be expected that the contribution of mentioned groups are different towards the values of electrostatic sensitivity. The number of amino groups attached to aromatic ring can increase the stability of energetic compounds. This effect was also indicated in deriving correlations for impact and shock sensitivity [17,21,22,28-32]. To find adjustable parameters, experimental data of electrostatic spark sensitivity for 17 nitro arene explosives with complex molecular structures, which are given in Table 1, were used as training set. The left-division method for solving linear equations uses the least squares method because the equation set is overdetermined [26] in using multiple linear regression method. Thus, optimized correlation has the following form:

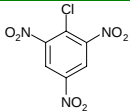
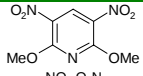
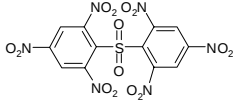
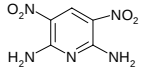
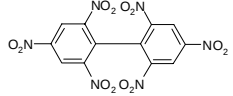
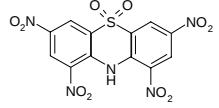
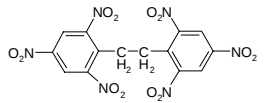
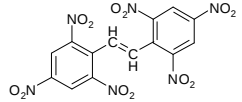
$$E_{ES} (J) = 28.18 - 3.052 D_{max} + 11.87 C_{SG} + 4.395 n_{-NH_2, -HNCO-} \quad (3)$$

Since the contribution of the variable C_{SG} is different for special groups, it can be determined as follows:

- a) $C_{SG} = 0.5$ for $-OH$ group attached to nitro arene ring, e.g. 2,4,6-trinitrophenol;
- b) $C_{SG} = 1.5$ for alkoxy group attached to nitroaromatic ring, e.g. 2-methoxy-1,3,5-trinitrobenzene;
- c) $C_{SG} = 0.25$ for $-N=N-$ and $-S(O_2)-$ groups attached to nitro arene ring, e.g. bis(2,4,6-trinitrophenyl)diazene.

Table 1. Comparison of estimated electrostatic sensitivity (J) of nitro arene compounds of training set with the measured data [11]

Name	Molecular structure	Molecular formula	$D_x(\text{km/s})$	C_{SG}	$n_{-NH_2, -NHCO-}$	$E_{ES}(\text{exp})$	$E_{ES}(\text{cal})$	Dev
Bis(2,4,6-trinitrophenyl)diazene (HNAB)		$C_{12}H_4N_8O_{12}$	7.47	0.25	0	8.2	8.30	-0.10
2,4,6-Trinitrobenzene-1,3-diol (TNR)		$C_6H_3N_3O_6$	7.64	0.5	0	12.3	10.77	1.53
2,4,6-Trinitrophenol (PA)		$C_6H_3N_3O_7$	7.56	0.5	0	8.98	11.00	-2.02
2-Methoxy-1,3,5-trinitrobenzene (TNA)		$C_7H_5N_3O_7$	7.14	1.5	0	28.59	24.15	4.44
2,4,6-Trinitrobenzene-1,3-diamine (DATB)		$C_6H_5N_5O_6$	7.85	0	2	10.97	12.96	-1.99
2,4,6-Trinitrobenzene-1,3,5-triamine (TATB)		$C_6H_6N_6O_6$	8.04	0	3	17.75	16.79	0.96
Bis(3-methyl-2,4,6-trinitrophenyl) diazene (DiMeHNAB)		$C_{14}H_8N_8O_{12}$	6.63	0.25	0	8.2	10.86	2.51
N,N'-Bis(2,4,6-trinitrophenyl) ethane-1,2-diamine (HNO)		$C_{14}H_6N_8O_{14}$	7.64	0	2	14.58	13.62	0.96

2-Chloro-1,3,5-trinitrobenzene (CTB)		<chem>C6H2N3O6Cl</chem>	7.60	0	0	6.71	4.95	1.76
2,6-Dimethoxy-3,5-dinitropyridine (DMDNPY)		<chem>C5H5N5O4</chem>	6.85	1.5	0	20.57	25.05	-4.48
1,3,5-Trinitro-2-[(2,4,6-trinitrophenyl) sulfonyl]benzene (DIPSO)		<chem>C12H4N6O14S</chem>	7.67	0.25	0	10.54	7.71	2.83
3,5-Dinitropyridine-2,6-diamine (DADNPY)		<chem>C5H5N5O6</chem>	7.90	0	2	12.4	12.81	-0.41
2,2',4,4',6,6'-Hexanitro-1,1'-biphenyl (HNB)		<chem>C12H4N6O12</chem>	7.52	0	0	5.03	5.19	-0.16
1,3,7,9-Tetranitro-10H-phenothiazine 5,5-dioxide (TNPTD)		<chem>C12H5N5O10S</chem>	6.97	0.25	0	5.78	9.85	-4.07
1,8-Dinitronaphthalene (1,8-DNN)		<chem>C10H6N2O4</chem>	5.92	0	0	13.9	10.06	3.84
1,3,5-Trinitro-2-[2-(2,4,6-trinitrophenyl) ethyl]benzene (DPE)		<chem>C14H8N6O12</chem>	6.68	0	0	3.89	7.75	-3.86
1,1'-(1,2-Ethenediyl)bis[2,4,6-trinitrobenzene] (HNS)		<chem>C14H6N6O12</chem>	6.90	0	0	5.32	7.07	-1.75

Due to the existence of different factors that can influence the electrostatic spark sensitivity of nitro arene compounds, R-squared value or the coefficient of determination of this correlation is 0.82 [26]. Electrostatic spark sensitivity of 17 nitro arene explosives as training set were also calculated by Eq. (3) and compared with the experimental values, which are shown in Table 1.

A visual comparison of the predictions with experiment for training set is also given in Fig. 1. As seen, the new method shows relatively good results as compared to experimental data.

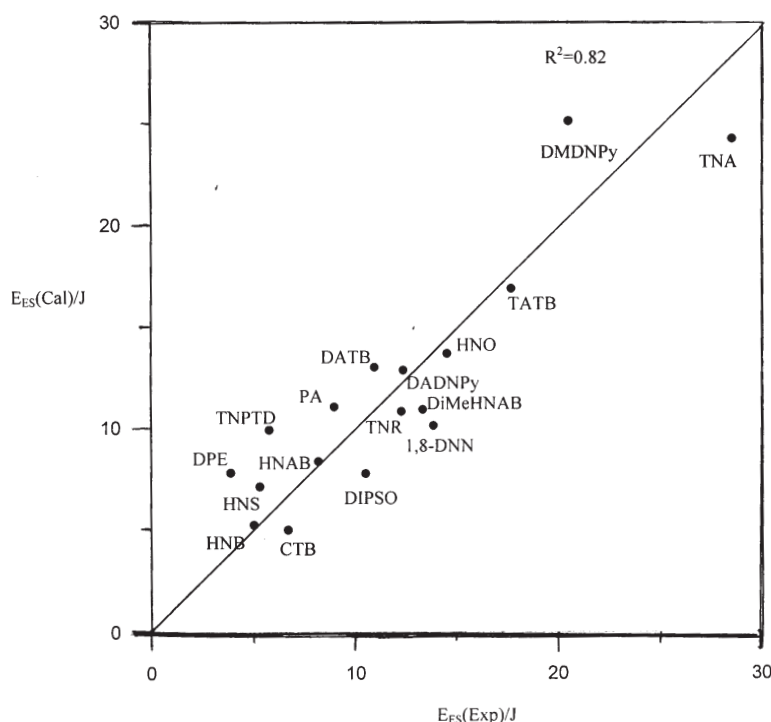


Fig. 1. Calculated electric spark sensitivity of training set versus experimental data for nitro arene energetic compounds. The solid lines represent exact agreement between predictions and experiment. Compound names for abbreviations are given in Table 1.

There is no unique idea of initiation mechanism of energetic materials by electric spark [9,33]. The primary fragmentation in this situation can be identical with the primary splitting process of low temperature thermolysis and detonation transformation of molecules of these materials [10]. The mechanism of energy transfer from electric spark to the reaction centre of molecule is not fully understood yet [9]. The idea of conversion of electric spark energy into a thermal effect has been suggested

by some authors [23,24]. One of the ways of specification of mechanism of the said energy spark energy transfer connects with the relationships between title sensitivity and some specific properties, e.g. thermal reactivity characteristics [9]. For all nitroaromatics given in Tables 1 and 2, on the whole the electric sensitivity increases with the increase the number of $-\text{NO}_2$ groups. As indicated in Eq. (3), the presence of $-\text{OH}$, $-\text{OR}$, $-\text{N}=\text{N}-$ and $-\text{S}(\text{O}_2)-$ groups as well as of the number of $-\text{NH}_2$ or $-\text{NHCO}-$ groups attached to aromatic ring can increase the value of E_{ES} on the basis of predicted D_{max} . However, some foundations about thermolysis of explosives with some mentioned groups are useful here. For $-\text{OH}$ group adjacent to nitro group, mechanism of thermolysis may involve migration of the said hydrogen to the oxygen of nitro group with subsequent homolysis of the $\text{N}-\text{OH}$ bond thus formed [9]. The primary thermolysis of some explosives, such as DIPSO and HNAB that contain $-\text{S}(\text{O}_2)-$ and $-\text{N}=\text{N}-$ groups, is not connected with reactivity of nitro group. It can be assumed that the $\text{C}-\text{S}$ and $\text{C}-\text{N}_2$ bonds are primarily split in the thermolysis of DIPSO and HNAB, respectively [9]. From the activation entropy values, it can also be assumed that the primary fragmentation of said explosives goes by cyclic mechanism [34].

4.2. Comparison of the results with quantum mechanical method

Wang and coworkers [13] have found the following correlation between electrostatic sensitivity and detonation velocity:

$$E_{\text{ES}} (J) = -0.3831D^2 + 27.68 \quad (4)$$

in which D is detonation velocity (km/s) that can be calculated by the Kamlet-Jacobs equation [15], i.e.

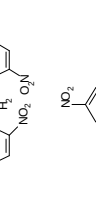
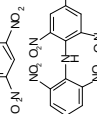
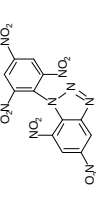
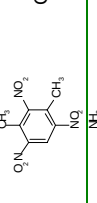
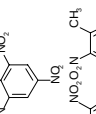
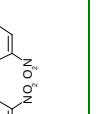
$$D = (NM^{1/2}Q^{1/2})^{1/2}(1.011 + 1.321\rho_0)$$

where ρ_0 is the packed density (g/cm³), M is an average molar weight of detonation products and Q is the estimated heat of detonation. They used the semi-empirical PM3 method [35] to compute heat of formation of explosive for calculation of Q . They were also carried out quantum chemistry computations by the Gaussian 98 program [36] with the DFT-B3LYP and basis set 6-31G* to obtain fully optimized molecular geometries [37,38]. Then, they have obtained the average molar volume and theoretical density using the Monte-Carlo method based on 0.001 electrons/bohr³ density space.

To test the reliability of the new correlation, electrostatic spark sensitivity for 17 nitro arene energetic compounds are also calculated and compared with measured values as well as computed results of Wang and coworkers, where Eq. (4) can be used, which are given in Table 2. As seen in Table 2, the root mean square (rms) deviations of Eq. (3) and Wang et al. [15] from experiment are 2.04 and 2.03 J,

Table 2. Comparison of estimated electrostatic sensitivity (J) of nitro arene compounds of test set with the measured data [11] as well as method of Wang and coworkers [13] on the basis of Kamlet-Jacobs detonation velocity (D_{K-J}) [15]

Name	Molecular structure	Molecular formula	$E_{ES}(exp)$	D_{K-J} (km/s)	E_{ES}^{ES} (Wang et al.)	Dev	D_{max} (km/s)	E_{ES} (cal)	Dev
1,3,5-Trimethyl-2,4,6-trinitrobenzene (TNMs)		$C_9H_9N_3O_7$	8.98	6.63	10.84	-1.86	6.23	9.12	-0.14
1,3,7,9-Tetranitro-10H-phenoxazine (TENPO)		$C_{12}H_5N_5O_9$	5.12	7.30	7.26	-2.14	7.30	7.11	-1.99
1,3,5-trinitro-2-[(2,4,6-trinitrophenyl)thio]benzene (DIPS)		$C_{12}H_4N_6O_{12}S$	2.56	8.01	3.10	-0.54	7.52	5.19	-2.63
2-Methyl-1,3,5-trinitro-4-[(2,4,6-trinitrophenyl)thio]benzene (MeDIPS)		$C_{13}H_6N_6O_{12}S$	5.71	7.92	3.65	2.06	7.10	6.47	-0.76
2-Methyl-4-[(3-methyl-2,4,6-trinitrophenyl)thio]-1,3,5-trinitrobenzene (DiMeDIPS)		$C_{14}H_8N_6O_{12}S$	8.57	7.62	5.43	3.14	6.68	7.75	0.82
2-Methyl-1,3,5-trinitrobenzene (TNT)		$C_7H_5N_3O_6$	6.85	7.37	6.87	-0.02	7.07	6.56	0.29
3-Methyl-2,4,6-trinitrophenol (TNCr)		$C_7H_5N_3O_7$	5.21	7.48	6.24	-1.03	7.14	6.34	-1.13

1,5-Dinitronaphthalene (1,5-DNN)		$C_{10}H_6N_2O_4$	11.2	5.64	15.49	-4.29	5.92	10.06	1.14
1,4,5-Trinitronaphthalene (TNN)		$C_{10}H_5N_3O_6$	10.97	6.70	10.48	0.49	6.48	8.37	2.60
1,4,5,8-Tetratronaphthalene (TENN)		$C_{10}H_4N_4O_8$	8.26	7.56	5.78	2.48	7.03	6.69	1.57
1,3,5-Trinitro-2-(2,4,6-trinitrobenzyl)benzene (DPM)		$C_{13}H_6N_6O_{12}$	4.1	7.74	4.73	-0.63	7.10	6.47	-2.37
1,3,5-Trinitrobenzene (TNB)		$C_6H_3N_3O_6$	6.31	7.68	5.08	1.23	7.49	5.29	1.02
N,N-Bis(2,4,6-trinitrophenyl)amine (DPA)		$C_{12}H_5N_7O_{12}$	5.02	7.97	3.34	1.68	7.70	4.63	0.39
5,7-Dinitro-1-(2,4,6-trinitrophenyl)-1H-1,2,3-benzotriazole (BTX)		$C_{12}H_4N_8O_{10}$	6.5	7.81	4.31	2.19	7.96	3.85	2.65
2,4-Dimethyl-1,3,5-trinitrobenzene (TNX)		$C_8H_7N_3O_6$	11.1	7.05	8.64	2.46	6.65	7.84	3.26
2,4,6-Trinitroaniline (PAM)		$C_6H_4N_3O_6$	6.85	7.67	5.14	1.71	7.38	10.02	-3.17
3,3'-Dimethyl-2,2',4,4',6,6'-hexanitro-1,1'-biphenyl (BtNT)		$C_{14}H_8N_6O_{12}$	4.28	7.52	6.01	1.73	6.68	7.75	-3.47
rms deviation			2.03						2.04

respectively. Thus, the rms deviations for both methods are nearly the same, which confirm the reliability of new correlation. A visual comparison of the predictions with experiment for new method and Wang et al. [15] is also given in Fig. 2. As seen, two methods show relatively good results with respect to measured values.

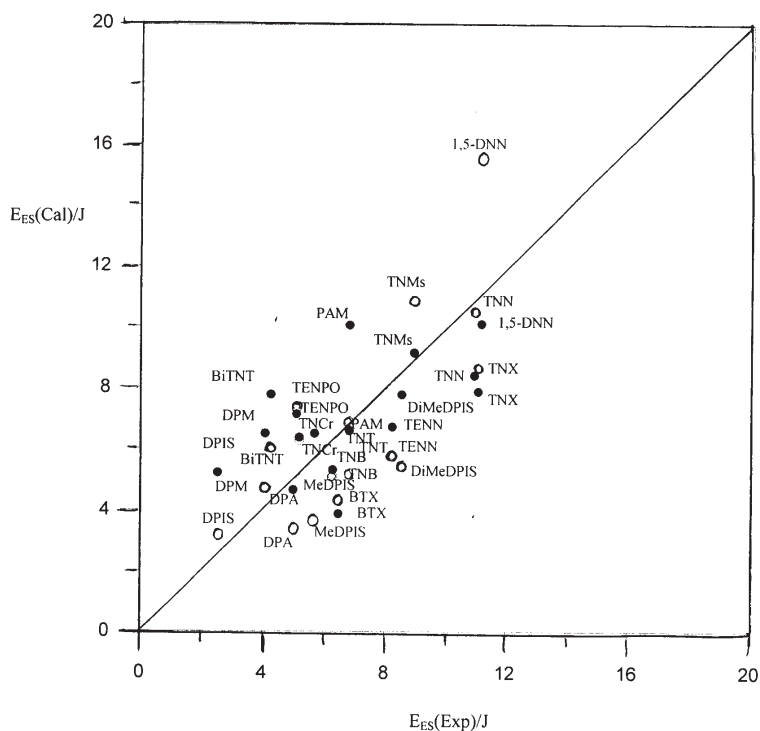


Fig. 2. Calculated electric spark sensitivity of test set versus experimental data for nitro arene energetic compounds. The solid lines represent exact agreement between predictions and experiment. Solid and hollow circles denote calculated electric spark sensitivity by Eq. (3) and Wang et al. method [13], respectively. Compound names for abbreviations are given in Table 2.

The calculated electrostatic spark sensitivity of 34 polynitroaromatic compounds of training and test sets, given in Tables 1 and 2, by new correlation are within 4.0 J of 31 measured values and more than 4.0 J for remainder 3 experimental data. Predictive ability of Eq. (3) may be taken as appropriate validation test of the new method for nitro arene compounds. Therefore, the results show that the accuracy of prediction is not necessarily enhanced by greater complexity.

4.3. Advantages of new correlation with respect to Wang et al. [15] method

Deviation of Wang et al. method [15] for some nitro arene energetic compounds are large as compared to calculated results of new method in Table 1, e.g. predicted values by Eq. (4) for TNA, TATB, HNO, DMDNPy and DIPSO are 6.01 J (Dev= 22.58 J), 4.67 J (13.08 J), 5.14 J (Dev = 9.44 J), 6.24 J (Dev = 14.33 J), and 1.03 J (Dev=9.51 J) respectively. Moreover, they have also found that Eq. (4) can not be applied for nitro arene explosives that contain some specific functional groups, e.g. -OH (such as PA).

One of the advantage of the new correlation is that Eq. (3) can also be used for nitro arene energetic compounds which have complex molecular structure, e.g. 5,7-dinitro-1-(2,4,6-trinitrophenyl)-1H-1,2,3-benzotriazole.

4.4. Limitations of new method

There are some limitations for new correlation: (i) It should be mentioned that the new method can predict electrostatic sensitivity close to the average value for some isomeric compounds where the difference of their sensitivities may be large. This situation can be attributed to different behavior of nitro groups in different positions. As representative example, predicted electrostatic spark sensitivity for dinitrobenzene is 6.97 J meanwhile the measured electrostatic spark sensitivity for 1,3-dinitrobenzene and 1,4-dinitrobenzene are 3.15 and 18.38 J [11], respectively; (ii) The new method can be used for secondary nitro arene explosives containing just C, H, N and O elements. Moreover, Eq. (3) can be used for those nitroaromatic explosives that do not contain N-NO₂ functional group because nitramines have different behavior [14]; (iii) The new correlation was derived for molecules with a detonation velocity between 6-8 km/s, and Eq. (3) may not be reliable for outside of this range.

5. Conclusions

This paper has introduced a new method for estimating the electrostatic spark sensitivities of nitro arene compounds as an important class of energetic compounds. New method is superior to complex quantum mechanical method in terms of accuracy, generality and simplicity. It uses detonation velocity at maximum nominal density of nitro arene and two structural parameters, which can be easily found.

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ПРОСТ НАЧИН ЗА ПРЕДВИЖДАНЕ НА ЕЛЕКТРОСТАТИЧНАТА ЧУВСТВИТЕЛНОСТ НА НИТРОАРОМАТНИ СЪЕДИНЕНИЯ

Резюме. В тази статия е описан прост начин за предвиждане на електростатичната чувствителност на нитроароматни съединения. Тази техника използва пресметнатите скорости на детонация при максимална плътност заедно с приноса на някои структурни параметри. Корелационната процедура е оптимизирана. Предсказаните резултати за 17 експлозива са сравнени с квантово-механични пресмятания. Съответствието на теоретичните пресмятания с експерименталните данни е добро.

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