Reliable prediction of electric spark sensitivity of nitramines: A general correlation with detonation pressure

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ABSTRACT

For nitramines, a general correlation has been introduced to predict electric spark sensitivity through detonation pressure. New method uses maximum obtainable detonation pressure as a fundamental relation so that it can be corrected for some nitramines which have some specific molecular structure. There is no need to use crystal density and heat of formation of nitramine explosives for predicting detonation pressure and electric spark sensitivity. The predicted electric spark sensitivities are compared with calculated results on the basis of quantum mechanical computations for some nitramines that latter can be applied. The root mean square (rms) deviations from experiment for new method and the predicted results of complicated quantum mechanical method are 1.18 and 3.49 J, respectively.

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1. Introduction

The advancement of empirical and computationally assisted design of new energetic materials will allow an estimate of their potential performance or possible hazards [1–3]. Although various parameters can affect to different kinds of sensitivities, some works have been done to predict sensitivity behavior of energetic materials [4,5]. As representative examples, some researches have been recently done to find general correlations for sensitivity of different classes of energetic materials on the basis of molecular structure of energetic compound [6–11]. Since detonation velocity and pressure of different energetic compounds can correlate with electric spark sensitivity, some authors have tried to find suitable correlations [12–16]. All of these methods have some restrictions such as they require crystal density and heat of formation of explosives to calculate the electric spark sensitivity through relationships of Kamlet and Jacobs method for prediction of detonation performance [17]. Moreover, derived correlations can be applied only for some specific groups of explosives. The purpose of this work is to determine a new correlation between electric spark sensitivity and detonation pressure of nitramine energetic compounds in which there is no need to use their crystal density and heat of formation. The paper introduces a simple pathway to find a reasonable good correlation for predicting electric spark sensitivity on the basis of new detonation

pressure relationship in which there is no need to use crystalline density and heat of formation of nitramines [18]. In this work, there is no need to use any experimental data or computed results in this new scheme. The predicted results will be compared with Wang et al. method [15] which uses complicated quantum chemistry computations for prediction of crystal density and heat of formation of nitramines. It will be shown that the predicted results are closer to the measured values as compared to Wang et al. method [15] for some nitramines that latter can be applied.

2. Theory

2.1. Initial knowledge about electric spark sensitivity

The electric spark or electrostatic sensitivity is defined as the degree of sensitivity to the electrostatic discharge which can be measured by the electrostatic discharge energy (E_{ES}) required for 50% initiation probability. Electric spark sensitivity depends on the configuration of the electrodes and structure of circuit so different results can be obtained by different test specification of electrode energy used by different authors [19]. An instrument marked as RDAD can be used to measure electric spark sensitivity for the secondary explosive class type in which the capacity of the capacitor is chosen so as to allow measurements in the voltage from 8 to 14 kV [5,19]. However, Zeman et al. have indicated [19] that there is a linear relationship between their experimental data of RDAD instrument with some of those obtained by the other methods of determination of the electric spark sensitivity in some recognized

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laboratories. It should be mentioned that the RDAD instrument is not suitable for determination of the sensitivity of primers and pyrotechnics [5] instead a new instrument, marked as ESZ KTTV [5,20], can be used for both primary and secondary explosives.

Since the mechanism of energy transfer from electric spark to the reaction center of molecule is not fully understood yet [12,13], there is no unique idea of initiation mechanism of energetic materials by electrostatic spark sensitivity. However, the primary fragmentation reactions in this initiation can be supposed identical with the primary splitting processes of low-temperature thermolysis [12,13]. The initiation can be considered as a multidisciplinary problem so that mechanism of the spark energy transfer can be related to molecular structure, thermal reactivity, sensitivity to mechanic stimuli and parameters of their detonation [12–14,21–23].

2.2. Relationship of electric spark sensitivity and performance

The first investigation was done by Zeman et al. [12–14] to find relationship between electric spark sensitivity and performance of explosives. They 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 electric spark sensitivity. Although they have shown that there was a linear relationship between the electric spark energy values and the squares of detonation velocities for some special groups of explosives, but there are no general correlations for different classes of explosives. Later, Wang et al. [15,16] also have tried to use quantum chemistry for prediction of crystal density of polynitroaromatic and nitramine energetic compounds. They have used the Gaussian 98 program [24] with the DFT-B3LYP and basis set 6-31G* to obtain fully optimized molecular geometries [25,26]. They have calculated the average molar volume and theoretical density using the Monte-Carlo method based on 0.001 electrons/bohr^3 density space. To correlate electric spark sensitivity with detonation performance, they used Kamlet and Jacobs correlations [17]. The Kamlet–Jacobs equation [17] for predicting detonation pressure can be given as follows:

$$P = 15.58\, NM^{0.5}Q_{\mathrm{det}}^{0.5}\rho_0^2 \tag{1}$$

where P is detonation pressure (kbar), ρ_0 is the packed density (g/cm^3), M is an average molar weight of detonation products an Q_{det} is the estimated heat of detonation. The Q_{det} can be obtained from the heat of decomposition of the explosive, defined as [17]:

$$Q_{\mathrm{det}} = \left(\frac{\Delta H_f(\mathrm{explosive}) - \Delta H_f(\mathrm{detonation\ products})}{\mathrm{formula\ weight\ of\ explosive}} \right) \tag{2}$$

If the heat of formation of the $C_aH_bN_cO_d$ explosive is known, Eq. (2) can be used to estimate heat of detonation. Wang et al. [15] used the semi-empirical PM3 method [27] to calculate heats of formation of nitramine energetic compounds. For a large number of nitramines with methylenenitramine units or $(-CH_2N(NO_2)-)$ in their molecules or with the better symmetrical nitramines but without methylenenitramine units, they have indicated that the following correlation exists between electrostatic sensitivity (E_{ES}) and detonation pressure for nitramine explosives [15]:

$$E_{ES}(J) = -76.92 \log P + 121.54 \tag{3}$$

Although Wang et al. [15] cited that Eq. (3) can be applied for nitramines with specified molecular structure; some nitramines without methylenenitramine units may have low deviations. However, this correlation has some limitations; i.e., (1) Eq. (3) is not a general correlation and it can not be applied for different nitramines, (2) the calculation of crystal density through quantum chemistry is complex and is not reliable for some cases, (3) the

computed gas phase heats of formation by PM3 rather than the condensed phase of formation of nitramines were used in Eq. (1) that can increase uncertainty in predicted detonation pressure and (4) deviations of predicted electric spark sensitivities are large for some nitramines with methylenenitramine units, e.g., DNDAH.

3. Results and discussion

It was recently found that it is possible to predict maximum obtainable detonation for any pure or mixed $C_aH_bN_cO_d$ explosives through the following equation [18]:

$$P' = 221.53 - 20.437a - 2.2538b + 17.216c + 16.140d$$
$$- 79.067C_{SSP} - 66.335n_N \tag{4}$$

where P' is maximum obtainable detonation pressure in kbar, C_{SSP} is equal to 1 for explosives which contain at least –N=N– or –O–NO$_2$ or NH$_4^+$ or –N$_3$ in the molecular structure and equal to zero for their absence, n_N is equal to $0.5n_{NO_2} + 1.5$ where n_{NO_2} is the number of nitro groups (–NO$_2$) attached to carbon in nitrocompounds in which $b = 1$. Eq. (4) provides a simple procedure for estimation of detonation pressure at maximum nominal or theoretical density. The study has shown that Eq. (4) and two specific structural parameters can be used to find a general correlation for E_{ES} of nitramines. It was found that two structural parameters have opposite effects in predicting E_{ES}. The following correlation can be used for this purpose:

$$E_{ES}(J) = x_1 + x_2 P' + x_3 SSP^- + x_4 SSP^+ \tag{5}$$

where SSP^- and SSP^+ are negative and positive contribution of specific structural parameters, respectively; x_1–x_4 are adjustable parameters which can be found from experimental data given in Table 1. The values of SSP^- and SSP^+ are equal to 1 or 0 for the presence or absence of these parameters in the molecular structure of nitramines. The parameters SSP^- and SSP^+ can be specified as follows:

(a) $SSP^- = 1$ for cyclic nitramines that contain only methylenenitramine units in which the number of CH$_2$–NNO$_2$ is less than or equal to 4, e.g., HMX, as well as acyclic nitramines which contain nitro or nitrate functional groups or $-(NO_2)N-C-C-N(NO_2)-$ fragment in their molecular structure.
(b) $SSP^+ = 1$ for the existence of specific molecular fragments such as –C–N–C– (in which N is not attached to NO$_2$), –C–O–C– in cyclic and acyclic nitramines, more than five nitramine groups and cyclic nitramines that contain $-(NO_2)N-C-C-N(NO_2)- \leq 2$.

To find adjustable parameters in Eq. (5), multiple linear regression method [28] was used. However, the left-division method for solving linear equations uses the least squares method because the equation set is overdetermined [28]. The optimized correlation can be given as follows:

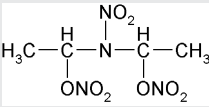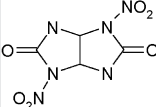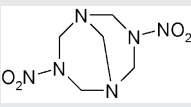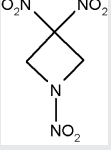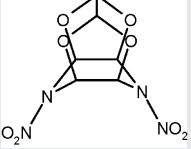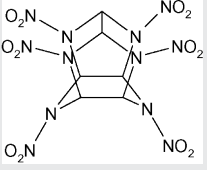$$E_{ES}(J) = 21.19 - 0.0422\, P' - 3.257\, SSP^- + 6.498\, SSP^+ \tag{6}$$

Fortunately, R-squared values or the coefficient of determination of Eq. (6) is 0.94 [28]. Predicted results for different nitramine energetic compounds are given in Table 1 and compared with measured values. The results are also compared with computed results of Wang et al. [15] for some nitramines that their method can be applied. As seen, the root mean square (rms) deviations of new method and Wang et al. [15] from experiment are 1.18 and 3.49 J, respectively. The contribution of SSP^+ in Eq. (6) is approximately twice of SSP$^-$ which has appreciable effect in the predicted values of E_{ES}. Thus increasing SSP^+ and decreasing SSP$^-$ can provide a suitable pathway for decreasing the electric spark sensitivity of nitramine energetic compounds.

Table 1
Comparison of predicted electric spark sensitivity (J) by new and Wang et al. [15] methods with the measured data for some nitramines that Eq. (3) can be applied.

Explosive	Molecular structure	P' (kbar)	E_{ES} (exp)	E_{ES} (Wang et al.)	Dev	E_{ES} (new)	Dev
RDX		346.8	2.49 [12]	2.47	0.02	3.29	−0.80
HMX		388.6	2.89 [12]	0.62	2.27	1.53	1.36
OCPX		243.3	13.45 [12]	14.15	−0.70	10.92	2.53
ORDX		317.4	8.08 [12]	9.15	−1.07	7.80	0.28
OHMX		359.1	5.5 [12]	7.69	−2.19	6.03	−0.53
TNAD		343.2	5.43 [12]	5.61	−0.18	6.71	−1.28
AcAn		332.9	13.93 [12]	13.88	0.05	13.59	0.34
DIGEN	$H_2C=N-NO_2$	263.3	8.38 [12]	11.20	−2.82	10.08	−1.70
DECAGEN		430.4	2.96 [12]	0.42	2.54	3.03	−0.07
DNDAH		225.7	12.49 [12]	23.28	−10.79	11.66	0.83
DNDC		255.2	15.97 [12]	15.83	0.14	16.87	−0.90
TETROGEN		305.1	6.25 [12]	4.25	2.00	5.06	1.19
TETRYL		282.4	5.49 [12]	–	–	6.01	−0.52
DMNO		292	5.49 [12]	–	–	5.61	−0.12
DMEDNA		250.7	8.24 [12]	–	–	7.35	0.89

Table 1 (*Continued*)

Explosive	Molecular structure	P' (kbar)	E_{ES} (exp)	E_{ES} (Wang et al.)	Dev	E_{ES} (new)	Dev
DINA		240.7	8.76 [12]	–	–	7.77	−1.91
DINGU		330.9	15.19 [12]	–	–	13.68	1.51
DPT		264.7	17.42 [12]	–	–	16.47	0.95
TNAZ		316.9	8.76 [5]	–	–	7.82	0.94
TEX		283.4	13.10 [5]	–	–	15.68	−2.58
CL-20		485.7	4.7 [5]	–	–	7.15	−2.45
rms deviation[a]					3.49		1.18

[a] For nitramines that Wang et al. method [15] can be applied.

For polynitronitramines, it was found that primary thermolysis occurs in homolytic splitting of N–N bond [12]. There are some relationships between E_{ES} and thermal decomposition parameters for some subgroups of nitamines [12]. The effect of molecular interactions through the molecular structure and its rigidity may be important. Since the number of intergrain contact points of nitramine grains in the volume unit is decreased by implantation of foreign particles, the addition of hard and fine admixture (crush glass or diamond dust) to RDX, HMX and Cl-20 can decrease the electric spark sensitivity of corresponding mixtures [20]. Besides, the effect of shape and size of nitramine crystals on E_{ES} might connect with dislocations in these crystals that influence a mechanism of energy transfer of the primary impulse into the reaction center of the given molecule [20]. There is an increase in the values of E_{ES} with the increasing grain size of HMX and RDX but two different behaviors were observed [20]. For example, there is an appreciable increasing of E_{ES} in RDX for some range of grain size with respect to HMX. Since there is no sufficient data and different behaviors of increasing the E_{ES} values with grain size of nitramines, the relationship of E_{ES} with the particle sizes of nitramine high energy materials cannot be incorporated in Eqs. (5) and (6). Increasing the E_{ES} values, when grain size of nitramines' crystals increase, can decrease the number of intergrain points in volume unit [21]. A brief survey of Zeman's results and some new correlations reveal the relationship between the electric spark sensitivity, detonation performance and activation energy of thermolysis of selected classes of energetic compounds with their molecular structures on the basis of different their behaviors [29–33].

The results confirm that new method has some advantages with respect to quantum mechanical computed values of Wang et al. [15] method: (i) new method can be applied for any nitramines and is not restricted to only nitramines with methylenenitramine units; (2) there is no need to use Gaussian program with appropriate basis set and PM3 method for prediction of crystal density and gas phase heat of formation, respectively; (3) the present method is much simple to use without using quantum mechanical methods which need high speed computer. Beside, the calculated results by new correlation are within ±3.0 J for all of data. However, new correlation is more easily to use and introduces reliable predicted results for some nitramines, e.g. predicted E_{ES} for DNDAH, as compared to Wang et al. [15] method. To apply new method for calculation of E_{ES} of new nitramine explosives, we have also considered two new nitramines TNAZ and TEX, where experimental data have been recently published [5]. The experimental data and the calculated values of E_{ES} for TEX and TNAZ as well as their molecular structures are given in Table 1. As seen in the molecular structures of TNAZ and TEX and Eq. (6), TNAZ does not have specific structure parameters (i.e. $SSP^+ = SSP^- = 0$) but TEX has –C–O–C– in its molecular structure (i.e. $SSP^+ = 0$ and $SSP^- = 1$). As indicated in Table 1, the calculated values for TEX and TNAZ are relatively close to the measured values.
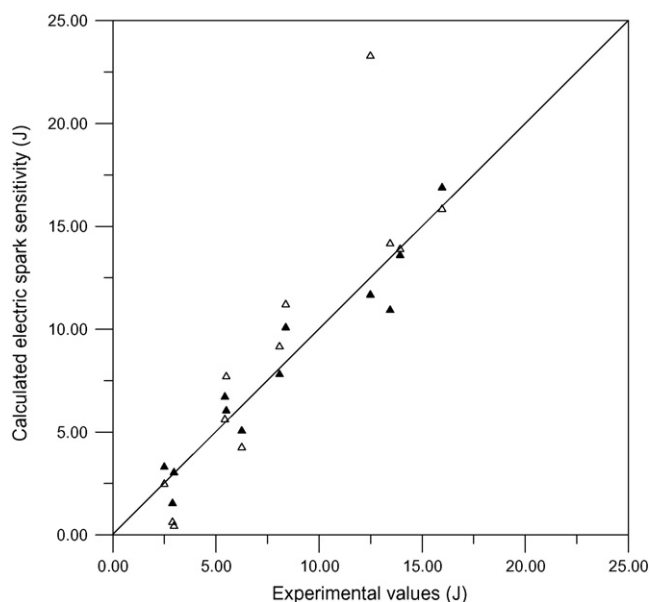
Fig. 1. Calculated electric spark sensitivity versus experimental data for nitramines. The solid lines represent exact agreement between predictions and experiment. Filled and hollow triangles denote calculated results of new method and Wang et al. [15], respectively.

Table 1 contains all experimental data for different nitramines where collected in Refs. [5] and [12]. Fig. 1 also shows a comparison of the calculated values of Eq. (6) and computed results of Wang et al. [15] with experimental values of nitramines for some nitramines that Eq. (3) can be applied. In this figure, exact agreement between the experiment and predicted values is presented by the line that bisects each figure along the diagonal. As evident in Fig. 1, new method shows relatively good agreement with experimental data, which may be taken as appropriate validation test of new method for nitramines.

4. Conclusions

Safe handling of novel energetic molecules is one of the most important issues to chemist who concern synthesis of energetic materials. Detonation pressure and electric spark sensitivity belong to important detonation and security characteristics of nitramines. Relationships between these two characteristics can be used for prediction of one parameter from the other. In the case of electric spark sensitivity the predictor model, presented in this paper, is showing up to be more easily for utility in practice compared to Wang et al. [15] method. Thus, new method is much simple for the chemist because it does not require complex quantum mechanical computer code as well as high speed computer. It should be mentioned that present method cannot be applied for the other classes of explosives which does not contain N–NO$_2$ functional group, e.g. 2,4-dinitroimidazole (2,4-DNI) and 2,4,6-trinitrobenzene-1,3,5-triamine (TATB).

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Glossary

AcAn: 2,4,6,8-tetranitro-2,4,6,8-tetraazanonane-1,9-diol diacetate
CL-20: 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo [5.5.0.0^{5,9}.0^{3,11}] dodcane
DECAGEN: 1,3,5,7,9-pentanitro-1,3,5,7,9-pentazecane
DIGEN: 1-nitro-1-azaethylene
DINA: N,N-bis(2-nitroxyethyl)-nitramine
DINGU: 1,4-dinitrotetrahydroimidazo[4,5-d]imidazole-2,5(1H,3H)-dione

DMEDNA: N,N′-dimethyl-N,N′-dinitroethane-1,2-diamine
DMNO: N,N′-dimethyl-N,N′-dinitroethanediamide
DNDAH: N,N-diethyl-N,N-dinitromethanediamine
DNDC: 1,4-dinitropiperazine
DPT: 3,7-dinitro-1,3,5,7-tetraazabicyclo [3.3.1] nonane
HMX: 1,3,5,7-tetranitro-1,3,5,7-tetrazocane
OCPX: 2,4-dinitro-2,4-diazapentane
OHMX: 2,4,6,8-tetranitro-2,4,6,8-tetraazanonane
ORDX: 2,4,5-trinitro-2,4,6-triazaheptane
RDX: 1,3,5-trinitro-1,3,5-triazinane
TETROGEN: 1,3-dinitro-1,3-diazetidine
TETRYL: N-methyl-N,2,4,6-tetranitroaniline
TEX: 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo [5.5.0.0^{5,9}.0^{3,11}] dodcane
TNAD: 1,4,5,8-tetranitrodecahydropyrazino[2,3-b]pyrazine
TNAZ: 1,1,3-trinitroazetidine