Research paper

A Novel Approach for the Prediction of Electric Spark Sensitivity of Polynitroarenes Based on the Measured Data from a New Instrument

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Abstract: This paper introduces two novel correlations for the assessment of the electric spark sensitivity of polynitroarenes based on a new instrument, marked as ESZ KTTV, which gives more reliable experimental data than a previous old system, marked as RDAD. The first correlation used the number of oxygen and chlorine atoms, as well as a correcting function that increases the predicted results based on elemental composition. Since the relationship between the measurements from ESZ KTTV and RDAD is not unequivocal, a second correlation can convert the reported data based on the RDAD system to the ESZ KTTV instrument. The second correlation can be applied to many available predictive methods, and provides the estimated results based on the RDAD instrument. For 34 polynitroarenes, where experimental values from both the RDAD and the ESZ KTTV instruments were available, the values of the root-mean-square deviation (RMSD) for the first and second correlations were 43.9 mJ and 36.0 mJ, respectively. Thus, due to the larger uncertainty in the measured data of the old RDAD system, both correlations provide more reliable data based on the ESZ KTTV instrument.

Keywords: electric spark sensitivity, RDAD, ESZ KTTV, polynitroarene, correlation

1　Introduction

Electric spark sensitivity is an important safety parameter for an energetic compound and indicates its degree of sensitivity to an electrical discharge. It was found that the output for electric spark sensitivity depends on the configuration of the electrodes, the general structure of the electrical circuit and finally on the discharge time [1-3]. These parameters are effective external variables, which depend on the kind of instrument used for the measurement of electric spark sensitivity [4-6]. Electric spark sensitivity depends also on other internal parameters, such as the chemical entity of a given material, its granulometry and grain shape, mechanical properties, temperature, moisture content, and its thermal and impact reactivities [3, 7, 8]. There are several different approaches and types of apparatus reported in the literature for measuring and solving electric spark sensitivity, where there is a linear relationship between the test results obtained with some apparatus types [9]. Among these instruments, two, marked as RDAD and ESZ KTTV, are especially important because there is much experimental data for two important types of secondary explosives, *i.e.* nitramines and polynitroarenes [2, 3, 8]. An analysis of the relationship between the outputs of these two instruments, RDAD and ESZ KTTV, revealed that the relationship is not unequivocal for nitramines and polynitroarenes [1-3]. Zeman *et al.* [1-3] concluded that the mechanisms of spark energy transfer into the reaction center of the molecule should be different in measurements on the RDAD and ESZ KTTV instruments. For the RDAD instrument, the thermal component of the discharge may be one of the reasons for this difference [2]. Large differences between the reported electric spark sensitivities from the RDAD and ESZ KTTV instruments support this assumption [2]. Thus, the considerable electrical energy losses for the area between the upper electrode and the sample surface contribute to higher values of electric spark sensitivity data on the RDAD instrument. Since the outputs of an RDAD instrument are connected with thermolysis of the given sample, large energetic losses in the spark gap of the RDAD instrument might manifest themselves as a strong thermal effect on the relevant electrical discharge [3]. Measurements by means of the ESZ KTTV system are more sensitive to the molecular structure of the studied polynitro compound than those from the RDAD instrument. This is due to the discharge in the spark gap in the RDAD system has passed through an air gap, whereas the electrode for the ESZ KTTV [2, 3] (*e.g.* in ESD 2008A [1]) is in direct contact with the sample. Considerable electrical energy losses occur in the air gap between the upper electrode and the sample surface in the old RDAD instrument.

Thus, a large part of the discharge is converted here into the expressive thermal component. Moreover, the RDAD instrument is not suitable for the determination of the sensitivity of primers and pyrotechnics.

Using the old RDAD instrument, Zeman *et al.* [10-13] reported the electric spark sensitivity of a large set of nitramines and polynitroarenes. These data have been used in recent years for the development of predictive methods for nitramines [14-19] and polynitroarenes [20-22]. Furthermore, the reported electric spark sensitivities based on the output from RDAD instruments have also been correlated with detonation performance [12, 23-26], impact sensitivity [27, 28], thermal stability [29-33], and shock sensitivity [34, 35]. Most of the available predictive methods and the new computer code EMDB [36] for the prediction of electric spark sensitivity are based on data reported for the old RDAD instrument. Today, the ESZ KTTV system is usually used in many laboratories for new energetic compounds, as well as for ionic liquids or salts. Some attempts have been made to correlate the output of the ESZ KTTV system for nitramines and polynitroarenes, as well as for ionic liquids, with some specific parameters [3, 37, 38]. The purpose of the present work is to introduce a simple general correlation for calculating the electric spark sensitivity of polynitroarenes based on their molecular structures, as well as to introduce a suitable correlation to convert the output from RDAD instruments to the ESZ KTTV system. The results of this work may be suitable for the extension of the output of previous work based on the RDAD instrument to the ESZ KTTV system.

2   Results and Discussion

2.1 Electric spark sensitivity based on the ESZ KTTV system and molecular structure of polynitroarenes

It has been shown that the elemental composition of some polynitroarenes play an important role in the assessment of their electric spark sensitivity based on the RDAD system [14, 19, 23]. A study of experimental data for various polynitroarenes based on the output from the ESZ KTTV system reveals that it is important to consider the contributions of some of the elemental compositions. For some polynitroarenes, it is essential to consider the presence of certain structural parameters because they can lower the estimated electric spark sensitivity based on part of the elemental composition. Table 1 shows the electric spark sensitivity of 34 different types of polynitroarenes with the general formula $C_aH_bN_cO_dCl_eS_f$ based on the RDAD and the ESZ KTTV systems, which have been collected by Zeman *et al.* [2].

Table 1. Comparison of the predicted electric spark sensitivity from the ESZ KTTV instrument by Equations 1 and 2 with experimental data [2]

| Name	RDAD [J]	ESZ KTTV [mJ]	Equation 1 [mJ]		Equation 2 [mJ]	
			Result	Dev.	Result	Dev.
1,3-Dinitrobenzene (1,3-DNB)	3.15	256.7	322.9	66.2	244.7	–12.0
1,4-Dinitrobenzene (1,4-DNB)	18.38	403.3	322.9	–80.4	403.1	–0.2
1,3,5-Trinitrobenzene (TNB)	6.31	108.2	173.1	64.9	138.2	30.0
2,2',4,4',6,6'-Hexanitrobiphenyl (HNB)	5.03	286.7	259.6	–27.1	264.3	–22.4
2,2',2'',4,4',4'',6,6',6''-Nonanitro-m-terphenyl (NONA)	16.44	158.2	212.2	54.0	243.5	85.3
1,8-Dinitronaphthalene (1,8-DNN)	13.90	238.2	189.0	–49.2	217.1	–21.1
1,5-Dinitronaphthalene (1,5-DNN)	11.20	180.0	189.0	9.0	189.0	9.0
1,4,5-Trinitronaphthalene (1,4,5-TNN)	10.97	210.0	173.1	–36.9	186.6	–23.4
1,4,5,8-Tetranitronaphthalene (TENN)	8.26	95.0	157.3	62.3	158.4	63.4
1-(2,4,6-Trinitrophenyl)-5,7-dinitrobenzotriazole (BTX)	6.50	135.0	141.5	6.5	140.1	5.1
2,4,6-Tris(2,4,6-trinitrophenyl)-1,3,5-triazine (TPT)	10.61	283.3	212.2	–71.1	322.3	39.0
1-Methyl-2,4,6-trinitrobenzene (2,4,6-Trinitrotoluene, TNT)	6.85	111.8	173.1	61.3	143.8	32.0
1,3,5-Trimethyl-2,4,6-trinitrobenzene (TNMs)	8.98	292.7	307.1	14.4	305.4	12.7
1-Amino-2,4,6-trinitrobenzene (PAM)	6.85	156.7	173.1	16.4	143.8	–12.9
1,3-Diamino-2,4,6-trinitrobenzene (DATB)	10.97	175.0	173.1	–1.9	186.6	11.6
1,3,5-Triamino-2,4,6-trinitrobenzene (TATB)	17.75	293.3	268.8	–24.5	257.2	–36.1

Name	RDAD [J]	ESZ KTTV [mJ]	Equation 1 [mJ]		Equation 2 [mJ]	
			Result	Dev.	Result	Dev.
2,4,6-Trinitrophenol (Picric acid, PA)	8.98	115.5	165.2	49.7	165.9	50.4
1,3-Dihydroxy-2,4,6-trinitrobenzene (TNR)	12.30	230.0	157.3	−72.7	200.5	−29.5
1-Methoxy-2,4,6-trinitrobenzene (2,4,6-Trinitroanisole, TNA)	28.59	436.0	452.3	16.3	369.9	−66.1
2-Chloro-1,3,5-trinitrobenzene (CTB)	6.71	101.0	102.1	1.1	80.3	−20.7
1,3-Dichloro-2,4,6-trinitrobenzene (DCTB)	2.55	31.5	31.0	−0.5	37.0	5.5
(E)-Bis(2,4,6-trinitrophenyl)diazene (HNAB)	8.20	112.0	125.7	13.7	95.8	−16.2
(E)-Bis(3-methyl-2,4,6-trinitrophenyl)-diazene (DMHNAB)	13.37	118.2	125.7	7.5	149.6	31.4
Bis(2,4,6-trinitrophenyl)sulfide (DIPS)	2.56	125.5	125.7	0.2	99.2	−26.3
Bis(2,4,6-trinitro-3-methylphenyl)sulfide (DMDIPS)	8.57	112.7	125.7	13.0	161.7	49.0
Bis(2,4,6-trinitrophenyl)sulfone (DIPSO)	10.54	186.7	262.9	76.2	182.2	−4.5
2,4,6-Trinitro-N-(2,4,6-trinitrophenyl)-aniline (DPA)	5.02	103.0	125.7	22.7	124.7	21.7
Bis-(2,4,6-trinitrophenyl)methane (DPM)	4.10	136.4	125.7	−10.7	115.2	−21.2
1,2-Bis-(2,4,6-trinitrophenyl)ethane (DPE)	3.89	167.0	125.7	−41.3	113.0	−54.0
3,3'-Dimethyl-2,2',4,4',6,6'-hexanitro-biphenyl (BITNT)	4.28	206.7	259.6	52.9	117.1	−89.6
2,6-Diamino-3,5-dinitropyridine (DADNP)	12.40	358.0	322.9	−35.1	340.9	−17.1
3,5-Dinitro-N,N'-bis(2,4,6-trinitro-phenyl)pyridine-2,6-diamine (PYX)	8.90	136.7	94.0	−42.7	165.1	28.4
1,3,7,9-Tetranitro-10H-phenothiazine 5-oxide (TNPTM)	10.68	195.0	149.4	−45.6	183.6	−11.4
1,3,7,9-Tetranitro-10H-phenothiazine 5,5-dioxide (TNPTD)	28.93	363.3	294.6	−68.7	373.5	10.2
Root-mean-square deviation				43.9		36.0

The multiple linear regression method [39] has been used to derive a new correlation as follows:

$$E_{ES,PNA}(ESZ\ KTTV) = 220.6 - 7.91d - 71.08e + 191.4E^+_{ES,PNA} \qquad (1)$$

where $E_{ES,PNA}(ESZ\ KTTV)$ is the electric spark sensitivity (in mJ) of polynitroarenes based on the ESZ KTTV system; d and e are equal to the number of moles of oxygen and chlorine atoms, respectively; $E^+_{ES,PNA}$ is a correcting function that increases the predicted result on the basis of d and e. Due to the uncertainty of the measured data, the R-squared values of the correlation from Equation 1 is relatively good, with $R^2 = 0.790$ [39]. The value of $E^+_{ES,PNA}$ is specified according to the following conditions (see Scheme 1):

a)   The presence of the molecular fragments (**1**) and (**2**), as well as the direct attachment of three alkyl groups or one aromatic ring to another aromatic ring and dinitrobenzene; for the presence of one of these molecular species, the value of $E^+_{ES,PNA}$ is equal to 0.7.

b)   The presence of three amino groups; the value of $E^+_{ES,PNA}$ is equal to 0.5.

c)   The presence of the group (**3**); the value of $E^+_{ES,PNA}$ is equal to 0.8.

d)   The presence of the molecular fragment (**4**); the value of $E^+_{ES,PNA}$ is equal to 1.5.

(1)   **(2)**   **(3)**   **(4)**
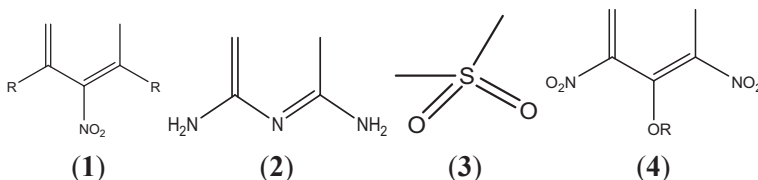
Scheme 1.   Molecular structures taken into consideration

2.2 Correlation between the output from the two instruments

It is valuable to correlate the results for the RDAD system with those for the ESZ KTTV instrument because most of the available predictive methods [40] and the new software EMDB [36] estimate the electric spark sensitivity based on the RDAD instrument. A study of the two different data sets has shown that there is a linear relationship between them for some polynitroarenes, but the presence of some molecular moieties may result in large deviations. Thus, it is possible to correlate them by considering some specific molecular fragments. Equation 2 gives this correlation, which was derived by the multiple linear regression method [39], as follows:

$$E_{ES,PNA}(ESZ\ KTTV) = 72.5 + 10.40E_{ES,PNA}(RDAD) + 139.4E^{+'}_{ES,PNA} - 62.03\ E^-_{ES,PNA} \quad (2)$$

where $E_{ES,PNA}(RDAD)$ is the electric spark sensitivity (in mJ) for polynitroarenes based on the RDAD system; $E_{ES,PNA}^{+'}$ and $E_{ES,PNA}^{-}$ are two correcting functions that can increase and decrease the predicted result based on the RDAD system, respectively. Due to the large uncertainty in the experimental values, R^2 is 0.859 [39]. The value of $E_{ES,PNA}^{+'}$ is equal to 1.0 for polynitroarenes under the following conditions:

a) The presence of the molecular fragment (**2**) and direct attachment of three alkyl groups to the aromatic ring, as well as dinitrobenzene.

b) Direct attachment of the picryl group to a triazene ring or to another picryl group.

The value of $E_{ES,PNA}^{-}$ is also equal to 1.0 for the presence of –N=N– or –Cl groups.

2.3 Statistical assessment of Equations 1 and 2

Statistical assessment of Equations 1 and 2 are given in Table 2, which includes regression coefficients, standard errors, *t*-statistics, *P*-values, as well as the upper and lower bounds of the 95% confidence interval. Standard errors provide the statistical significance of the regression coefficients in predicting the values of the electric spark sensitivity in both equations.

Table 2. Regression coefficients, standard errors, *t*-statistics, *P*-values, and confidence intervals for the new models

Model	Variable	Coefficient	Standard error	*t*-statistic	*P*-value[a]	Lower bound (95%)[b]	Upper bound (95%)[c]
Equation 1	Intercept	220.6	21.2	10.40	1.83E-11	177.3	263.9
	D	−7.91	2.06	−3.843	0.00059	−12.12	−3.71
	E	−71.08	22.11	−3.215	0.00312	−116.24	−25.93
	$E_{ES,PNA}^{+}$	191.4	20.8	9.202	3.06E-10	148.9	233.9
Equation 2	Intercept	72.5	13.8	5.259	1.12E-05	44.4	100.7
	$E_{ES,PNA}(RDAD)$	10.40	1.08	9.668	9.98E-11	8.20	126.0
	$E_{ES,PNA}^{+'}$	139.4	17.5	7.959	6.96E-09	103.6	175.2
	$E_{ES,PNA}^{-}$	−62.03	20.93	−2.964	0.0059	−104.76	−19.29

[a] Probability of rejecting a true null hypothesis; [b] Lower bound of the 95% confidence interval; [c] Upper bound of the 95% confidence interval.

A variable in Equations 1 and 2 is significant if the standard error is small relative to its coefficient. Since the *t*-statistic is the ratio of the coefficients to their standard errors, higher values of the *t*-statistic correspond to the more

significant coefficients [41, 42]. The *P*-value of a variable shows the probability that the parameter predicted from the measured data should have the value that was determined. The *P*-value for each term tests the null hypothesis that the coefficient is equal to zero (no effect). The null hypothesis can be rejected for a low *P*-value (<0.05). Thus, the effect is significant and the observed effect is not due to random variations for this situation [43]. These statistical assessments show that the proposed three descriptors in Equations 1 and 2 have a highly significant ability to predict $E_{ES,PNA}$*(ESZ KTTV)*. The root-mean-square deviation (RMSD) measures the differences between the values predicted by a model and the measured data. As seen in Table 1, the values of RMSD for Equations 1 and 2 are 43.9 mJ and 36.0 mJ, which confirms the greater reliability of Equation 2 as compared to Equation 1. Figure 1 also shows a graphical comparison between the new models, where the predictions of Equation 2 exhibit a lower dispersion with respect to Equation 1. This situation is consistent with the higher R^2 and lower RMSD values of Equation 2.
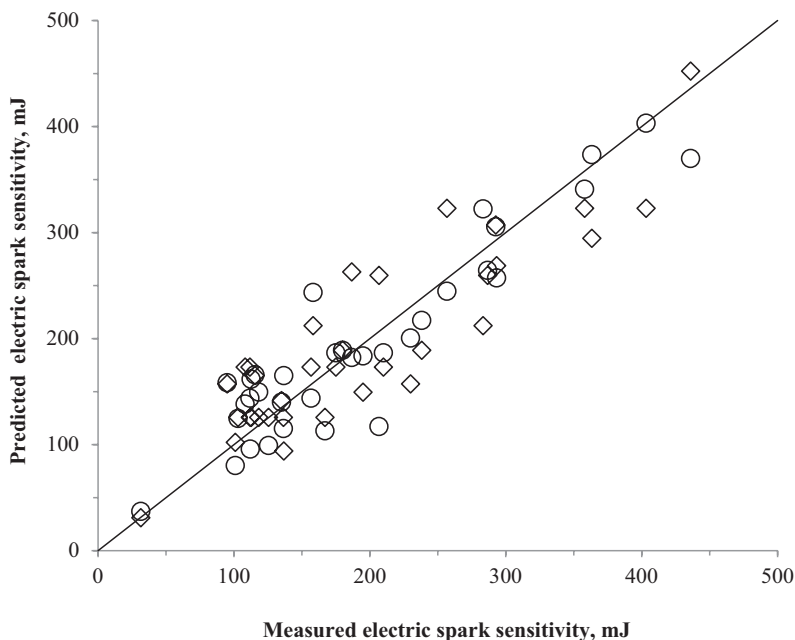
Figure 1.   The predicted electric spark sensitivity using two novel correlations versus the experimental values for 34 polynitroarenes: ◊ – Equation 1, ○ – Equation 2, straight line – best fit (linear)

3   Conclusions

Two new correlations have been introduced for desk calculation of the electric spark sensitivity of polynitroarenes based on the ESZ KTTV system from their molecular structures and $E_{ES,PNA}(RDAD)$. The first correlation uses the number of oxygen and chlorine atoms as well as a correcting function $E^+_{ES,PNA}$ that increases the predicted results based on elemental composition. The second correlation can covert the predicted results of previously available methods, which were based on $E_{ES,PNA}(RDAD)$ data, to the electric spark sensitivity based on the ESZ KTTV system. Due to the presence of larger uncertainties for the old RDAD system with respect to the ESZ KTTV instrument, both correlations provide better predictions than those previously available that were based on the old RDAD system.

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