

Prediction of impact sensitivity of nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives

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Abstract

This paper describes a new method for prediction of impact sensitivity of nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives. The new procedure is based on some structural parameters of $C_aH_bN_cO_d$ explosives. Three essential parameters would be needed in this scheme which contain $a + b/2 - d$ and the number of nitrogens as well as the number of $R-C(NO_2)_2-CH_2-$ structural parameters attached to oxygen of carboxylate functional groups where R is alkyl groups. The results are compared with experimental data and some empirical correlations. Predicted impact sensitivities for 58 explosives have a root mean square (rms) of deviation from experiment of 27 cm, which show good agreement with respect to measured values as compared to previous empirical models.

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1. Introduction

Detonation performance and sensitivity of explosives are two important parameters for explosive industries. Detonation pressure, heat of detonation, detonation velocity and temperature are important performance detonation parameters for measuring the effectiveness of ideal and non-ideal explosives. They are predicted using a complicated computer code such as CHEETAH [1] or different empirical methods [2,3]. As representative example, some new methods have also been recently introduced to predict detonation velocity for ideal and non-ideal explosive through different simple paths [3–11]. Shock and impact are two well-known of many kinds of sensitivity [2]. Drop weight test is a test to evaluate impact sensitivity by which milligram quantities of an explosive material are placed between a flat tool steel anvil and the flat surface of a tool striker. Some drops are usually made by a 2.5 kg weight for different heights so that the height in centimeter, at which the probability of explosion is 50%, is denoted by H_{50} . The results of drop weight impact measurement are not often reproducible and give widely varying H_{50} values in some cases. Some works have been done to relate impact sen-

sivities to various molecular features, structural and electronic properties [12–52].

Since safe handling is one of the most important issues to the scientists and engineers who handle energetic molecules, sensitivity prediction of significant importance in deriving novel energetic molecules. Impact sensitivity is closely related to many accidents in working places among various aspects of sensitivity. The purpose of this work is to predict a simple correlation for the impact sensitivity of nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives. This impact sensitivity calculation was conducted for 58 polynitroaliphatic and the other classes of explosives to compare against experimental results as well as a new correlation [50] and Kamlet and Adolph [12,13] method. It is shown here how this method can predict good results on impact sensitivity and screening of notional energetic materials as compared to the more complex computer output, e.g. quantum mechanical computations [48]. The most important aspect of the present work is that only three structural parameters are necessary to directly determine impact sensitivity.

2. Some methods for determination of impact sensitivities

The nature of impact sensitivity test, obtaining reliable experimental data is known to be relatively difficult. This difficulty

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is probably associated with puzzles in initiation mechanism of explosion caused by mechanical impact because it is believed that hot spots in the material contribute to initiation in the drop weight impact test. Moreover, factors in the impact experiment that might affect the formation and growth of hot spots could affect the measurements. Therefore, impact sensitivity tests are very much dependent on tests condition. The impact test is considered to provide only a crude and qualitative estimate of an explosive's sensitivity. Despite all of the uncertainties associated with the impact test, most studies that have attempted to associate molecular properties with sensitivities rely on drop weight impact measurements. Some simple correlations have been found which relate impact sensitivities with molecular properties such as the oxygen balance of molecules [12,13], molecular electronegativities [23,24], vibrational states [32,39], molecular weights and detonation gas concentrations [18], parameters related to oxidation numbers [25], partial atomic charges [14–16,39,21,27], heat of reaction [40], heat of explosion [22], activation energies [22,37,38,41,42,46] and bond order [38,41,42].

High-speed computers allow quantum mechanical calculations of individual molecules so that many macroscopic properties of bulk energetic materials can be predicted using quantum mechanical information for isolated molecules. It was noted that molecular surface of electrostatic potentials of the nitroaromatic molecules have positively charged regions over the C–NO₂ bonds. Politzer and coworkers [19,20,34–36,43] used this unusual feature to suggest that the C–NO₂ bond in nitroaromatic systems might serve as a site for nucleophilic attack. They have also identified a few features of electrostatic potential surrounding an isolated molecule for CHNO explosives that appear to be related to their impact sensitivity [19,20,21,27,34–36,43]. Owen et al. [21] undertook an investigation to address whether the electrostatic potential over the C–NO₂ bonding region reflects a degree of instability in the C–NO₂ bond that would subsequently indicate the sensitivity of the explosive. Murray et al. [27] also found a correlation between impact sensitivity measurements and an approximation of the electrostatic potential at the midpoint of C–N bond for 18 nitroaromatics that did not include hydroxynitroaromatic molecules. Rice and Hare [48] developed five models using parameters related to features of the surface electrostatic potentials. Their predictions support the Murray et al. [33,43] observations that the impact sensitivities of CHNO explosives have some dependence on the degree of internal charge imbalance within the molecule. Although quantum mechanical calculations have a stronger theoretical basis for prediction of sensitivity of explosives, simple empirical correlations have the advantages that neither complex quantum chemistry software such as the Gaussian 98 [53] nor high-speed computers need to be available for tedious computation.

Some new methods have also been introduced to calculate impact sensitivities. Neural networks architectures have been recently used as prediction methodology for impact sensitivity to cover various types of energetic molecules. Cho et al. [49] utilized 17 molecular descriptors, which were composed of compositional and topological descriptors in an input layer

and two hidden neurons in a hidden layer. It was also found that the artificial neural network can be used to determine impact sensitivity of explosives by choosing only 10 molecular descriptors [51]. Moreover, it was shown that elemental composition of CHNO explosives can be used to predict impact sensitivities of selected class of explosives [50]. The predicted results by this scheme [50] can give good outputs as compared to five quantum mechanical models of Rice and Hare [48]. Furthermore, a generalized method has been introduced to evaluate impact sensitivity of various nitroheterocycles of practical importance including nitropyridines, nitroimidazoles, nitropyrzoles, nitrofurazanes, nitrotriazoles and nitropyrimidines [52]. The number of –CNC– and –CNNC– moieties in aromatic ring as well as the elemental compositions was used in this method. The results for 69 heterocyclic compounds were compared with complex neural networks computations of Cho et al. which showed 58 and 71 cm for new correlation and neural networks computations methods respectively [52].

3. New method for prediction of impact sensitivity

Oxygen content of explosives is one of the essential parameter to determine impact sensitivity. Kamlet and Adolph [12,13] assessed impact sensitivity through correlation of oxygen balance, which can be defined as $OB_{100} = 100(2n_O - n_H - 2n_C - 2n_{COO})/MW$, where n_O , n_H , n_C , n_{COO} are the number of oxygen, hydrogen, carbon and carboxylate in the molecule, respectively, and MW is the molecular weight of explosive. They were used OB_{100} to find some linear correlations between OB_{100} and $\log H_{50}$ for some classes of explosives including nitroaliphatics as follows:

$$\log H_{50} = 1.74 - 0.23OB_{100} \quad (1)$$

It was recently found that elemental composition can also be used to predict different classes of explosives [50], close to classifications which were done by Kamlet and Adolph [12,13], so that the following correlation can be applied for any $C_aH_bN_cO_d$ polynitroaliphatics:

$$\log H_{50} = \frac{81.40a + 16.11b - 19.08c + 1.089d}{MW} \quad (2)$$

where MW is the molecular weight of polynitroaliphatic energetic compound.

It is proposed here that application of oxygen content and some structural parameters can be used to find reliable correlation for impact sensitivity of nitroaliphatic, nitroaliphatic containing other functional groups and nitrate energetic compounds. The results indicated that the following general equation with some structural parameters is suitable for mentioned compounds:

$$\log H_{50} = y_1 + y_2 \left[\frac{100(a + b/2 - d)}{MW} \right] + y_3 \left[\frac{100c}{MW} \right] + y_4 n_{R-C(NO_2)_2-CH_2-} \quad (3)$$

where y_1 – y_4 are adjustable coefficients which can be obtained by the best fit to experimental impact sensitivities data for differ-

Table 1
Comparison of new correlation, Eq. (4), with experimental data [29] as well as calculated values of K–P [50] and K–A [12,13] methods for nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives

Energetic compound	Formula	$n_{R-C(NO_2)_2-CH_2-}$	$(H_{50})_{exp}$	Eq. (4)	Dev.	K–A	Dev.	K–P	Dev.
1,1,1,3-Tetranitrobutane	C ₄ H ₆ N ₄ O ₈	0	33	32	1	32	1	31	2
1,1,1,3,5,5-Heptanitropentane	C ₅ H ₅ N ₇ O ₁₄	0	8	9	-1	6	2	9	-1
1,1,1,6,6,6-Hexanitro-3-hexyne	C ₆ H ₄ N ₆ O ₁₂	0	7	17	-10	13	-6	19	-12
1,1,1,6,6,6-Hexanitro-3-hexene	C ₆ H ₆ N ₆ O ₁₂	0	17	22	-5	18	-1	23	-6
3,3,4,4-Tetranitrohexane	C ₆ H ₁₀ N ₄ O ₈	0	80	144	-64	235	-155	154	-74
2,2,4,4,6,6-Hexanitroheptane	C ₇ H ₁₀ N ₆ O ₁₂	0	29	48	-19	55	-26	50	-21
2,2,4,6,6-Pentanitroheptane	C ₇ H ₁₁ N ₅ O ₁₀	0	56	102	-46	148	-92	109	-53
2,2,2-Trinitroethylcarbamate	C ₃ H ₄ N ₄ O ₈	0	18	13	5	17	1	12	6
2,2-Dinitro-1,3-propanediol	C ₃ H ₅ N ₂ O ₆	0	110	77	33	55	55	73	37
Methyl-2,2,2-trinitroethyl carbonate	C ₄ H ₅ N ₃ O ₉	0	28	30	-2	24	4	32	-4
4,4,4-Trinitrobutyramide	C ₄ H ₆ N ₄ O ₇	0	40	39	1	55	-15	39	1
Bis-(2,2,2-trinitroethyl)-carbonate	C ₅ H ₄ N ₆ O ₁₅	0	16	9	7	5	11	9	7
Methylene-bis- <i>N,N'</i> -(2,2,2-trinitroacetamide)	C ₅ H ₄ N ₈ O ₁₄	0	9	7	2	6	3	7	2
Bis-(trinitroethoxy)-methane	C ₅ H ₆ N ₆ O ₁₄	0	17	12	5	7	10	12	5
<i>N,N'</i> -Bis-(2,2,2-trinitroethyl)-urea	C ₅ H ₆ N ₈ O ₁₃	0	17	10	7	10	7	9	8
5,5,5-Trinitropentanone-2	C ₅ H ₇ N ₃ O ₇	0	125	116	9	132	-7	134	-9
Ethyl-2,2,2-trinitroethyl carbonate	C ₅ H ₇ N ₃ O ₉	0	81	66	15	71	10	74	7
<i>N</i> -(2-propyl)-trinitroacetamide	C ₅ H ₈ N ₄ O ₇	0	112	92	20	164	-52	95	17
Bis-(trinitroethyl)-oxalate	C ₆ H ₄ N ₆ O ₁₆	0	15	11	4	6	9	12	3
2,2,2-Trinitroethyl-4,4,4-trinitrobutrate	C ₆ H ₆ N ₆ O ₁₄	0	18	17	1	14	4	18	0
Bis-(trinitroethyl)-oxamide	C ₆ H ₆ N ₈ O ₁₄	0	13	12	1	12	1	12	1
Trinitroethyl-2,2-dinitropropylcarbonate	C ₆ H ₇ N ₅ O ₁₃	1	15	41	-26	22	-7	29	-14
<i>N</i> -Trinitroethyl-4,4,4-trinitrobutramide	C ₆ H ₇ N ₇ O ₁₃	0	18	18	0	17	1	18	0
1,5-Bis-(trinitroethyl)-biuret	C ₆ H ₇ N ₉ O ₁₄	0	24	12	12	14	10	11	13
<i>N</i> -(<i>t</i> -Butyl)-trinitroacetamide	C ₆ H ₁₀ N ₄ O ₇	0	110	194	-84	433	-323	210	-100
Tris-(2,2,2-trinitroethyl)-orthoformate	C ₇ H ₇ N ₉ O ₂₁	0	7	9	-2	6	1	9	-2
1,1,1,7,7,7-Hexanitroheptanone-4	C ₇ H ₈ N ₆ O ₁₃	0	34	33	1	28	6	36	-2
Methylene-bis-(trinitroethyl)-carbamate	C ₇ H ₈ N ₈ O ₁₆	0	27	17	10	18	9	17	10
2,2-Dinitropropyltrinitrobutyrate	C ₇ H ₉ N ₅ O ₁₂	1	151	83	68	66	85	60	91
2,2,2-Trinitroethyl-4,4-dinitrovalerate	C ₇ H ₉ N ₅ O ₁₂	0	70	54	16	66	4	60	10
Bis-(2,2-dinitropropyl)-carbonate	C ₇ H ₁₀ N ₄ O ₁₁	2	300	228	72	121	179	111	189
2,2-Dinitropropyl-4,4,4-trinitrobutyramide	C ₇ H ₁₀ N ₆ O ₁₁	0	72	57	15	79	-7	60	12
Bis-(trinitropropyl)-urea	C ₇ H ₁₀ N ₈ O ₁₃	0	23	28	-5	40	-17	27	-4
Bis-(1,1,1-trinitro-2-propyl)-urea	C ₇ H ₁₀ N ₈ O ₁₃	0	19	28	-9	40	-21	27	-8
Bis-(trinitroethyl)-fumarate	C ₈ H ₆ N ₆ O ₁₆	0	14	25	-11	23	-9	30	-16
Trinitroethyl-bis-(trinitroethoxy)-acetate	C ₈ H ₇ N ₉ O ₂₂	0	6	11	-5	7	-1	11	-5
4,4,4-Trinitrobutyric anhydride	C ₈ H ₈ N ₆ O ₁₅	0	30	34	-4	30	0	39	-9
Bis-(2,2,2-trinitroethyl)-succinate	C ₈ H ₈ N ₆ O ₁₆	0	30	30	0	31	-1	35	-5
Bis-(2,2-dinitropropyl)-oxalate	C ₈ H ₁₀ N ₄ O ₁₂	2	227	249	-22	164	63	131	96
<i>N,N'</i> -Bis-(3,3,3-trinitropropyl)-oxamide	C ₈ H ₁₀ N ₈ O ₁₄	0	45	32	13	41	4	34	11
2,2,2-Trinitroethyl-4,4-dinitrohexanoate	C ₈ H ₁₁ N ₅ O ₁₂	0	138	92	46	132	6	105	33
2,2-Dinitrobutyl-4,4,4-trinitrobutramide	C ₈ H ₁₁ N ₅ O ₁₂	0	101	92	9	93	8	105	-4
2,2-Dinitropropyl-4,4-dinitrovalerate	C ₈ H ₁₂ N ₄ O ₁₀	1	320	327	-7	402	-82	254	66
Nitroisobutyl-4,4,4-trinitrobutrate	C ₈ H ₁₂ N ₄ O ₁₀	0	279	213	66	270	9	254	25
Tetrakis-(2,2,2-trinitroethyl)-orthocarbonate	C ₉ H ₈ N ₁₂ O ₂₈	0	7	8	-1	5	2	8	-1
Methylene-bis-(4,4,4-trinitrobutramide)	C ₉ H ₁₂ N ₈ O ₁₄	0	113	50	63	97	16	54	59
Ethylene-bis-(4,4,4-trinitrobutrate)	C ₁₀ H ₁₂ N ₆ O ₁₆	0	120	71	49	95	25	85	35
<i>N,N'</i> -Bis-(2,2-dinitropropyl)-4,4,4-trinitrobutramide	C ₁₀ H ₁₄ N ₈ O ₁₅	0	72	67	5	93	-21	72	0
Bis-(2,2,2-trinitroethyl)-4,4-dinitroheptanedioate	C ₁₁ H ₁₂ N ₈ O ₂₀	0	68	40	28	44	24	46	22
2,2-Dinitropropane-1,3-diol-(4,4,4-trinitrobutrate)	C ₁₁ H ₁₂ N ₈ O ₂₀	0	50	40	10	44	6	46	4
Bis-(2,2,2-trinitroethyl)-4,4,6,6,8,8-hexanitro-undecanedioate	C ₁₅ H ₁₆ N ₁₂ O ₂₈	0	32	33	-1	34	-2	38	-6
1,2,3-Propanetriol trinitrate	C ₃ H ₅ N ₃ O ₉	0	20	18	2	8	12	17	3
<i>N</i> -(2,2,2-trinitroethyl)-nitraminoethyl nitrate	C ₄ H ₆ N ₆ O ₁₁	0	7	12	-5	11	-4	10	-3
2,2-Bis-(nitroxymethyl)-1,3-propanediol dinitrate	C ₅ H ₈ N ₄ O ₁₂	0	13	32	-19	16	-3	31	-18
3-[<i>N</i> -(2,2,2-trinitroethyl)-nitramino]-propyl nitrate	C ₅ H ₈ N ₆ O ₁₁	0	12	23	-11	25	-13	21	-9
3,5,5-Trinitro-3-azahexyl nitrate	C ₅ H ₉ N ₅ O ₉	0	21	48	-27	69	-48	44	-23
1,9-Dinitrato-2,4,6,8-tetranitrazanonane	C ₅ H ₁₀ N ₁₀ O ₁₄	0	10	10	0	17	-7	8	2
4,4,8,8-Tetranitro-1,11-dinitrato-6-nitrazo undecane	C ₁₀ H ₁₆ N ₈ O ₁₆	0	87	70	17	92	-5	72	15
rms deviation (cm)					27		60		40

ent $C_aH_bN_cO_d$ energetic compounds, $a + b/2 - d$ is a parameter that shows distribution of oxygen between carbon and hydrogen to form carbon monoxide and water, $n_{R-C(NO_2)_2-CH_2-}$ is the number of $R-C(NO_2)_2-CH_2-$ structural parameters attached to oxygen of carboxylate functional groups where R is alkyl groups. The parameter $100(a + b/2 - d)/MW$ is a good factor to show oxygen content of energetic compound [10]. The second parameter is related to pervious work [50] which shows the contribution of nitrogen atoms in determining sensitivity. Moreover, the extra stability was found in Table 1 for some polynitroaliphatics that contain $R-C(NO_2)_2-CH_2-$ structural parameters attached to oxygen of carboxylate functional groups. It can be expected that optimized adjustable coefficients y_4 has positive value. To obtain adjustable coefficients, a database given by Storm et al. [29] were used such that experimental values of impact sensitivity for a variety of molecules had been collected. Since measured data of impact sensitivity varies widely with instrumental types and conditions of the experiment, the database of Storm et al. [29] was not augmented by others. Multiple linear regression method [54] was used to find adjustable coefficients. The left-division method for solving linear equations uses the least squares method because the equation set is overdetermined [54]. The optimized correlation can be given as following:

$$\log H_{50} = 2.47 + 0.371 \left[\frac{100(a + b/2 - d)}{MW} \right] - 0.485 \left[\frac{100c}{MW} \right] + 0.185n_{R-C(NO_2)_2-CH_2-} \quad (4)$$

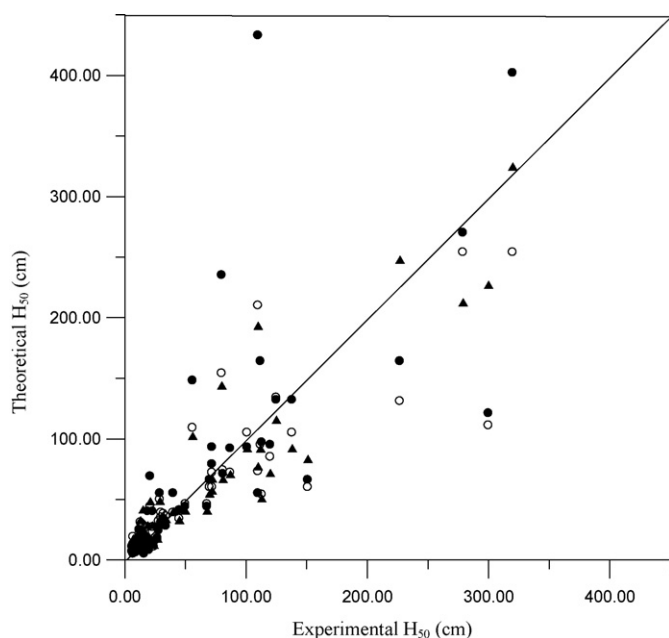


Fig. 1. Predicted impact sensitivity of nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives vs. experimental values. The solid lines represent exact agreement between predictions and experiment. Solid and hollow circles denote calculated heats of detonation by K–A and K–P methods, respectively. Filled triangles denote calculated results of new method.

Measured data of Table 1 were used to find adjustable coefficients of Eq. (3). Predicted impact sensitivities by new correlation for 58 of nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives are given in Table 1. The results are also compared with calculated values of Keshavarz and Pouretedal (K–P) [50] as well as Kamlet and Adolph (K–A) [12,13] methods. As indicated in Table 1, the results show a good agreement with experimental values (rms = 27 cm) as compared to K–P (rms = 40 cm) and K–A (rms = 60 cm) methods. Comparison of calculated results with experimental data listed in Table 1 may be taken as appropriate validation of the new simple correlation for use with $C_aH_bN_cO_d$ nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives. A visual comparison of the predictions with experiment is given in Fig. 1. As evident in Fig. 1, the new method shows the best agreement with experimental data.

4. Conclusions

Since high percentage of error is observed in reported experimental measurements from different sources, the main intent in this work was to investigate the likelihood of a generalized method to evaluate impact sensitivity of nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives. Therefore, a new reliable method to predict the impact sensitivity of mentioned energetic compounds has been presented. Eq. (4) can predict reliable results as compared to the best available empirical methods. The new procedure requires only structural formula of organic polynitroaliphatics.

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