

## Simple empirical method for prediction of impact sensitivity of selected class of explosives

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### Abstract

A new approach is described in this work to predict impact sensitivity of a variety of polynitroaliphatics, polynitroaromatics and the explosives containing N-NO<sub>2</sub>. This paper introduces some simple correlations for prediction of impact sensitivity of C<sub>a</sub>H<sub>b</sub>N<sub>c</sub>O<sub>d</sub> explosives using *a*, *b*, *c*, *d*, molecular weight and structure information of the explosive. The new correlations are applied to test different polynitroaromatics, benzofuroxans and nitramines. The results are compared with experimental data and some models of complex quantum mechanics computation. Predicted impact sensitivities for 46 explosives have a root mean square (rms) of deviation from experiment of 24 cm, which show good agreement with respect to measured values as compared to five different quantum mechanical models. Impact sensitivities for 58 polynitroaliphatics and related explosives are also calculated, and have a rms deviation from experiment of 40 cm. © 2005 Elsevier B.V. All rights reserved.

**Keywords:** Impact sensitivities; C<sub>a</sub>H<sub>b</sub>N<sub>c</sub>O<sub>d</sub> explosives; Correlations; Detonation; Safety

### 1. Introduction

The performance and sensitivity parameters of a new energetic material are very important because its development, manufacture, testing and fielding is cost effective, environmentally desirable and time saving capabilities. Some properties such as toxicity and melting point are also needed ultimately widely used a new candidate energetic material, but initial research effort is guided by trinity of the performance and sensitivity. The idea of judging the potential safety of use an explosive is essential in various its application. The study of explosives by theoretical methods has provided a considerable insight for identification of promising and elimination of candidates for additional consideration. Detonation heat, pressure and velocity for explosives and specific impulse for propellants are used in evaluating potential energetic systems. The heat of reaction during detonation process,

the pressure and the rate of propagation of the shock wave front through material are important detonation parameters, which can be used to determine the performance of explosives [1]. Specific impulse is a measure of thrust that can be related to detonation velocity for high explosives [2], they can be designated as monopropellant in this case, and combustion temperature by a simple procedure to assess the performance of propellants [3]. All of the mentioned quantities depend on energy release during detonation and combustion process.

A sophisticated computational network, e.g. TIGER computer code [4], as well as an equation of state for detonation products, such as the Jacobs–Cowperthwaite–Zwisler equation of state (JCZ–EOS) [5,6], Becker–Kistiakosky–Wilson equation of state (BKW–EOS) [1] and Kihara–Hikita–Tanaka equation of state (KHT–EOS) [7], are usually used for determination of detonation parameters. Numerous empirical methods have also been introduced for simple prediction detonation performance of explosives. Some studies have been recently provided different approaches for predicting detonation parameters of different classes of explosives,

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which can determine reliable performance of energetic materials by simple correlations [8–13].

Numerous studies have been done to relate impact sensitivities to various molecular features, structural and electronic [14–50]. They correlate impact sensitivities with direct and indirect molecular properties such as oxygen balance, electronegativity, vibrational states, partial atomic charge, etc. Of the different methods for calculation of impact sensitivities, the method of Kamlet and Adolph [14–17] can be easily applied for large classes of explosives through oxygen balance so that they are very interesting for chemists. On the other hand, quantum mechanical methods recently applied in the variety of predictive methodologies used in assessing energetic materials, e.g. a quantum mechanical determination of the relation between impact sensitivity and the charge distribution in energetic molecules [50].

There is a continuing need in the field of energetic materials for reliable predictions sensitivity of energetic materials in order to increase safety. The purpose of this work is to show a simple approach for predicting the impact sensitivity of different classes of  $C_aH_bN_cO_d$  explosives. It should be noted that the accuracy of predictive method is not necessarily enhanced by greater complexity, e.g. quantum mechanical methods. This method for calculation impact sensitivity will be applied to some polynitroaromatic, benzofuroxan and nitramines  $C_aH_bN_cO_d$  explosives for showing the reliability of the predicted values against experiment as compared to complex quantum mechanical models of Rice and Hare [50] as well as Kamlet and Adolph [14–17] method. We will also investigate the interrelationships between impact sensitivity of large number of polynitroaliphatic and the other classes of explosives to show the reliability of present correlations. The most important aspect of the present work is that only the values of  $a$ ,  $b$ ,  $c$  and  $d$  are sufficient directly to determine sensitivity of many  $C_aH_bN_cO_d$  explosives. Although quantum mechanical calculations have a stronger theoretical basis for prediction of sensitivity of explosives, the introduced empirical procedure introduced in this work has the advantages that neither complex quantum chemistry software such as the Gaussian 98 [51] nor high speed computers needs to be available for tedious computation. The new procedure presented herein show that this method to predict impact sensitivity of different classes  $C_aH_bN_cO_d$  explosives is a very simple computational tool to be used for quick calculation and screening of notional energetic materials with about the same reliability as one might attach to the more complex computer output.

## 2. Initial knowledge of impact sensitivities

One of the important factors in assessing an explosive is its vulnerability to detonation caused by accidental impact or shock. Several properties contribute to explosive response to the stimulus in a sensitivity test, namely the ease with which a detectable relation of any kind and a high-order detonation as well as tendency of a small reaction can be initiated and

established in an explosive. Some of stimuli can cause detonation, which includes impact, shock, heat, electrostatic charge and friction. Of these, shock and impact are two well known of many kinds of sensitivity so that the drop weight impact test is extremely easy to implement. A standard small-scale gap test [52] is often used to measure shock sensitivity. Since measurements using shock sensitivity tests have been done for small number of pure explosives, finding a correlation between molecular properties and reliable shock sensitivity data is difficult. Drop weight test is one of the tests for evaluation impact sensitivity. The drop weight impact test is convenient method 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, explosion or non-explosion are recorded. Explosion is distinguished at an arbitrarily set level of sound, which is produced by the explosive on impact. The height in centimetres, at which the probability of explosion is 50%, is denoted by  $h_{50}$ . Since initiation by impact is extremely complicated, reported data serve only as approximation indication of sensitivity. The results of drop weight impact measurement are not often reproducible and give widely varying  $h_{50}$  values in some cases. Organic explosives can undergo very rapid and high exothermic reaction for which an understanding of sensitivity is in large part of chemical problem. Since all explosives are necessarily metastable and sensitive, maximizing performance while minimizing sensitivity is highly desirable in designing and formulating of energetic materials. It is desirable to have an ideal explosive with high performance as well as insensitive enough to permit safer handling. Due to difficulty of initiation of detonation process, an explosive should not be so insensitive. Theoretical studies of energetic materials have provided a considerable insight into understanding of factors affecting their behavior.

Of numerous studies of correlations of impact sensitivities with various molecular features, structural and electronic, Kamlet and Adolph [14–17] introduced a very simple conventional scheme that can be applied to large number explosives. In their work the impact sensitivity is linearly related to a measure of oxygen balance by the following equation:

$$\log h_{50} = a_1 + a_2 \text{OB}_{100} \quad (1)$$

the constants  $a_1$  and  $a_2$  have different values for four classes of  $C_aH_bN_cO_d$  explosives, namely nitroaromatic with  $\alpha$ -CH and without  $\alpha$ -CH, nitroaliphatic and nitramine. Values of  $a_1$  and  $a_2$  in Eq. (1) are positive and negative, respectively, for the various classes of explosives, which shows the more impact sensitive explosives are those with more positive  $\text{OB}_{100}$ . Oxygen balance,  $\text{OB}_{100}$ , is a procedure of quantifying how well an explosive provides its own oxidant so that it can be balanced in terms of oxidant per 100 g  $C_aH_bN_cO_d$  explosive as follows:

$$\text{OB}_{100} = \frac{2d - b - 2c - 2n(\text{CO}_2)}{\text{MW}} \quad (2)$$

where  $n(\text{CO}_2)$  is the numbers  $\text{CO}_2$  moieties, e.g. in esters or carboxylic acids, that are contained in the molecule and MW is the molecular weight of explosive.

High speed computers allow quantum mechanical calculations of individual molecules so that many macroscopic properties, such as aqueous salvation free energies, lattice energies in ionic crystals, diffusion coefficients, solubilities, heats of vaporization, boiling points, partition coefficients, crystal constants and impact sensitivities [53–61], of bulk materials can be determined. Rice and Hare [50] developed five models using parameters related to features of the surface electrostatic potentials, which can be summarized as below:

*Model 1:* The approximate electrostatic potential at the midpoint of each bond,  $\bar{V}_M$ , is evaluated using the partial charges for all atoms in the molecule rather than only the two atoms of carbon and nitrogen making up the bond C–N in C–NO<sub>2</sub> which earlier was described by Murray et al. [37]. This presentation of  $\bar{V}_M$  is

$$\bar{V}_M = \frac{1}{N} \sum_{i=1}^N \sum_j^n \frac{q_j}{r_{ij}} \quad (3)$$

where  $n$  is the number of atoms in the molecule,  $N$  the number of bonds in the molecule for which electrostatic potentials of midpoints of the bonds were calculated,  $q_j$  the partial charge on each atom and  $r_{ij}$  is the distance from the midpoint of the  $i$ th bond to the  $j$ th atom. The function with best-fit parameters for calculation of  $h_{50}$  in this case is described as:

$$h_{50}(/cm) = 63.6 + 1.89 \times 10^4 \times \exp(-0.0879 \text{ mol/kcal} \times \bar{V}_M) - 0.3675 \text{ mol/kcal} \times \bar{V}_M \quad (4)$$

*Model 2:* This model is based the difference between the magnitudes of the averages of the positive and negative values of the electrostatic potential on the isosurface [40],  $|\bar{V}^+ - |\bar{V}^-||$ , that is shown as:

$$h_{50}(/cm) = 9.2 + 8.03 \times 10^2 \times \exp\left[-\left(0.366 \text{ mol/kcal} \times |\bar{V}^+ - |\bar{V}^-||\right)\right] \quad (5)$$

*Model 3:* This model depends on another statistical quantity associated with the electrostatic potential of the molecule, the balance parameter  $\nu$  [37,40] so that the non-linear least-squares fit of the data to the following equation:

$$h_{50}(/cm) = 29.3 + 1.386 \times 10^{-3} \times \exp[48.84 \times \nu] \quad (6)$$

*Model 4:* The generalized interaction property function (GIPF) methodology using quantum mechanical information about a single molecule can be used to evaluate heats of detonation,  $Q_{\text{det}}$  [62]. A non-linear least-squares fit of the data

to the function:

$$h_{50}(/cm) = 27.8 + 0.1135 \times \exp\left[-\left(11.079 \text{ g/kcal} \left[Q_{\text{det}} - 1.661 \text{ kcal/g}\right]\right)\right] \quad (7)$$

*Model 5:* This model uses the exponential dependencies of both the GIPF balance parameter  $\nu$  and heats of detonation [62] in the following function:

$$h_{50}(/cm) = 1.341 \times \exp\left(8.1389\nu - 6.7922 \text{ g/kcal} \left[Q_{\text{det}} - 1.4737 \text{ kcal/g}\right]\right) \quad (8)$$

Rice and Hare [50] in their work described limitations of mentioned models for describing  $h_{50}$  in various explosives.

### 3. A simple approach for determining impact sensitivity

It is proposed here that application of some empirical correlations to explosives comprised of C, H, N and O have resulted simple relationships between impact sensitivity and elemental composition. The results indicated that the following general equation is suitable for different categories of  $\text{C}_a\text{H}_b\text{N}_c\text{O}_d$  explosives with four adjustable parameters:

$$\log h_{50} = \frac{A_1 a + B_1 b + C_1 c + D_1 d}{\text{MW}} \quad (9)$$

where  $a$ ,  $b$ ,  $c$  and  $d$  are stoichiometric coefficients for an explosive of general formula  $\text{C}_a\text{H}_b\text{N}_c\text{O}_d$ , MW the molecular weight of the explosive and  $A_1$ ,  $B_1$ ,  $C_1$  and  $D_1$  are the values to be adjusted to obtain the best fit to experimental impact sensitivities data for different classes of explosives. This equation provides the basis for the simplest method of estimation of impact sensitivities, which requires as input information only the elemental composition. The results showed that following classifications of explosives are suitable for prediction of impact sensitivities:

- polynitroaromatics (and benzofuroxans);
- polynitroaromatics with  $\alpha$ -CH and  $\alpha$ -N-CH (e.g. tetryl) and nitramines;
- polynitroaliphatics.

These divisions are close to classifications, which were done by Kamlet and Adolph [14–17]. The results of various studies showed that explosives belong to one of the mentioned classes can have similar behavior, based on the introduced general correlation of Eq. (9), for calculation of impact sensitivities. Since the effect of the formation and growth of hot spots in the material could strongly affect the measurements of initiation in the drop weight impact test [50], the results of impact test are often not reproducible and give widely varying  $h_{50}$  values, e.g. reported  $h_{50}$  values for twice-recrystallized

2,4,6-trinitrotoluene vary below 100 to above 250 cm [50]. Due to the apparent sensitivity of the results to conditions of experiment, there is a concern as to the quality of the experimental data of drop weight impact measurements to be used in establishing correlations. Drop weight impact tests that were performed under the same machine and the same operator are suitable in establishing correlations between chemical composition of the explosive and measured data for which

conditions of the tests were unvarying, well-defined and controlled. To find the constants of Eq. (9), experimental impact sensitivities of polynitroaromatic were selected only from collected values of Rice and Hare [50] that are based on evaluated data by Wilson et al. [44], while for the second and third classes, reported data of Storm et al. [43] are also added to obtain suitable correlations. The results show that three optimized correlations (9a)–(9c) can be obtained for above

Table 1

Experimental  $h_{50}$  and measured values of new correlations, Kamlet and Adolph [14–17] (K–A), five models of Rice and Hare [50] for explosives

Explosive <sup>a</sup>	Experimental <sup>b</sup>	New	Dev	K–A	Dev	Model 1		Model 2		Model 3		Model 4		Model 5	
						Model	Dev	Model	Dev	Model	Dev	Model	Dev	Model	Dev
HNB	11	12	-1	3	8	14	-3	34	-23	29	-18	28	-17	1	10
PNB	11	18	-7	5	6	18	-7	17	-6	29	-18	28	-17	2	9
TetNB	28	33	-5	13	15	25	3	20	8	30	-2	31	-3	7	21
TNB	71	80	-9	50	21	38	33	39	32	43	28	56	15	52	19
Picric acid	64	66	-2	28	36	48	16	52	12	51	13	76	-12	77	-13
PNA	22	30	-8	7	15	27	-5	17	5	29	-7	29	-7	4	18
TetNA	47	58	-11	17	30	39	8	34	13	32	15	36	11	19	28
TNA	141	147	-6	61	80	97	44	89	52	90	51	125	16	141	0
DATB	320	250	70	73	247	259	61	214	106	200	120	283	37	301	19
TATB	490	399	91	86	404	501	-11	498	-8	307	183	502	-12	478	12
HNBP	70	42	28	38	32	25	45	33	37	32	38	43	27	26	44
DIPAM	67	80	-13	47	20	41	26	83	-16	43	24	77	-10	72	-5
DNBF	76	44	32	36	40	54	22	40	36	57	19	31	45	14	62
Picryl azide	19	47	-28	34	-15	38	-19	52	-33	37	-18	33	-14	17	2
CL-16	17	15	2	5	12	20	-3	32	-15	29	-12	28	-11	1	16
Styphnic acid	43	56	-13	17	26	62	-19	62	-19	48	-5	113	-70	106	-63
ADNBF	100	80	20	45	55	91	9	87	13	100	0	42	58	45	55
CL-14	120	138	-18	54	66	182	-62	198	-78	285	-165	67	53	102	18
CL-17	56	37	19	14	42	43	13	58	-2	31	25	30	26	7	49
CL-18	56	47	9	34	22	98	-42	84	-28	93	-37	30	26	15	41
BTF	53	16	37	21	32	70	-17	32	21	30	23	28	25	1	52
HNS	54	71	-17	81	-27	50	4	33	21	34	20	60	-6	47	7
tri245	68	30	38	5	63	22	46	19	49	29	39	30	38	4	64
24-DNI	105	95	10	21	84	61	44	34	71	32	73	59	46	41	64
Methyl picrate	192	187	5	73	119	80	112	86	106	98	94	108	84	128	64
2,3,4,5-TetNT	15	37	-22	92	-77	35	-20	24	-9	32	-17	37	-22	19	-4
2,3,4,6-TetNT	19	37	-18	92	-73	34	-15	30	-11	31	-12	38	-19	20	-1
2,3,5,6-TetNT	25	37	-12	92	-67	31	-6	30	-5	32	-7	38	-13	20	5
2,4,6-TNT	98	95	3	521	-423	64	34	73	25	80	18	133	-35	143	-45
2,3,4-TNT	56	95	-39	521	-465	92	-36	107	-51	131	-75	92	-36	119	-63
3,4,5-TNT	107	95	12	521	-414	71	36	103	4	208	-101	100	7	140	-33
TetN- <i>o</i> -Tol	36	38	-2	116	-80	60	-24	29	7	31	5	49	-13	30	6
TetN- <i>m</i> -Tol	37	38	-1	116	-79	57	-20	66	-29	43	-6	52	-15	47	-10
TetN- <i>p</i> -Tol	47	38	9	116	-69	57	-10	63	-16	34	13	50	-3	38	9
HNDPM	39	54	-15	206	-167	42	-3	34	5	32	7	59	-20	41	-2
Tetryl	25	38	-13	40	-15	42	-17	48	-23	38	-13	45	-20	34	-9
(MeNO <sub>2</sub> N)-22	21	32	-11	82	-61	33	-12	23	-2	30	-9	36	-15	14	7
(MeNO <sub>2</sub> N)-23	18	32	-14	82	-64	34	-16	34	-16	33	-15	37	-19	20	-2
PNT	18	19	-1	27	-9	24	-6	23	-5	29	-11	30	-12	4	14
14-DNI	55	17	38	21	34	80	-25	227	-172	262	-207	36	19	38	17
PETN	13	21	-8	16	-3	88	-75	28	-15	30	-17	41	-28	16	-3
$\epsilon$ -CL20	12	10	2	23	-11	45	-33	16	-4	29	-17	29	-17	3	9
$\beta$ -CL20	14	10	4	23	-9	71	-57	16	-2	29	-15	29	-15	3	11
RDX	28	20	8	55	-27	314	-286	49	-21	31	-3	39	-11	22	6
HMX	32	20	12	55	-23	152	-120	21	11	31	1	41	-9	22	10
EDNA	34	40	-6	130	-96	1066	-1032	69	-35	45	-11	190	-156	153	-119
rms Deviation (cm)			24		142		162		43		59		37		35

<sup>a</sup> See Glossary for glossary of compound names and chemical formulas.

<sup>b</sup> All  $h_{50}$  values were taken from collected data of Rice and Hare [50].

Table 2

Experimental  $h_{50}$  [43] and calculated values of Kamlet and Adolph [14–17] (K–A) and new correlation for nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives

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

classification of explosives, respectively:

$$\log h_{50} = \frac{11.76a + 61.72b + 26.89c + 11.48d}{MW} \quad (9a)$$

$$\log h_{50} = \frac{47.33a + 23.50b + 2.357c - 1.105d}{MW} \quad (9b)$$

$$\log h_{50} = \frac{81.40a + 16.11b - 19.08c + 1.089d}{MW} \quad (9c)$$

Impact sensitivities estimated by these correlations for some explosives are given in Table 1 and compared with values calculated from five models of Rice and Hare [50] as well as Kamlet and Adolph [14–17] and measured values. As indicated in Table 1, the new correlations of  $h_{50}$ , in contrast to the method of Kamlet and Adolph [14–17], show surprisingly good agreement with experimental values and give good results as compared to complex quantum mechanical computation. Since all of mentioned explosives in Table 1 follow Eqs. (9a) and (9b), calculated values of  $h_{50}$  by Eq. (9c) for nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives are also given in Table 2 and compared with the calculated values of Kamlet and Adolph [14–17]. Comparison of calculated results with experimental data listed in Tables 1 and 2 may be taken as appropriate validation of the new simple correlations for use with  $C_aH_bN_cO_d$  explosives. It is worthwhile to note that the present method is very simple and at the same time, gives results that are comparable to those from other more complex quantum mechanical methods. Since lower particle size explosive materials are more sensitive than explosives with higher particle size, the experimental data on the impact sensitivity of lower particle size differs from the higher particle size. Moreover, the explosive with needle shape may be more sensitive and hazardous than round shape, which cannot be considered in this work.

#### 4. Conclusions

The methodology presented here have several advantages: (a) neither experimental data nor further information except the explosive's composition need to be measured or estimated for calculating impact sensitivities; (b) there is no need to obtain oxygen balance of molecule, molecular electronegativities, vibrational states, molecular weights and detonation gas concentrations, parameters related to oxidation numbers, partial atomic charges, heats of reaction, heats of explosion, activation energies, bond order, the electrostatic potentials, and the other parameters which are usually required previous studies [14–50]; (c) the correlations are much simple for rapid desk calculation of impact sensitivities with about the same reliance on their answers as one could use complicated methods; (d) introduced correlations comprise board classes of  $C_aH_bN_cO_d$  explosives, i.e. polynitroaromatic, bezofuroxan, polynitroaliphatic, Polynitroaromatic with  $\alpha$ -CH and  $\alpha$ -N-CH (e.g. tetryl) and nitramine.

In brief, the new correlations were introduced here for simply hand calculating impact sensitivities of board classes of  $C_aH_bN_cO_d$  explosives that require only the explosive's composition. The new procedure is also simple in form and easy to use in a practical sense.

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## Glossary of compound names and molecular formulas

- ADNBF*: C<sub>6</sub>H<sub>3</sub>N<sub>5</sub>O<sub>6</sub>; 7-amino-4,6-dinitrobenzofuroxan.
- BTF*: C<sub>6</sub>N<sub>6</sub>O<sub>6</sub>; benzotrifuroxan.
- ε-CL-20*: C<sub>5</sub>H<sub>8</sub>N<sub>4</sub>O<sub>12</sub>; 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (ε-polymorph).
- β-CL-20*: C<sub>5</sub>H<sub>8</sub>N<sub>4</sub>O<sub>12</sub>; 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (β-polymorph).
- CL-16*: C<sub>6</sub>N<sub>8</sub>O<sub>10</sub>; azidopentanitrobenzene.
- Styphnic acid*: C<sub>6</sub>H<sub>3</sub>N<sub>3</sub>O<sub>8</sub>; 2,4,6-trinitroresorcinol.
- CL-14*: C<sub>6</sub>H<sub>4</sub>N<sub>6</sub>O<sub>6</sub>; 5,7-diamino-4,6-dinitrobenzofuroxan.
- CL-17*: C<sub>6</sub>H<sub>2</sub>N<sub>6</sub>O<sub>8</sub>; 7-amino-4,5,6-trinitrobenzofuroxan.
- CL-18*: C<sub>6</sub>H<sub>2</sub>N<sub>6</sub>O<sub>6</sub>; 8-amino-7-nitrobenzobisfuroxan.
- DATB*: C<sub>6</sub>H<sub>5</sub>N<sub>5</sub>O<sub>6</sub>; 1,3-diamino-2,4,6-trinitrobenzene.
- DIPAM*: C<sub>12</sub>H<sub>6</sub>N<sub>8</sub>O<sub>12</sub>; 3,3'-diamino-2,2',4,4',6,6'-hexanitrobiphenyl.
- DNBF*: C<sub>6</sub>H<sub>2</sub>N<sub>4</sub>O<sub>6</sub>; 2,2',3,3',4,4',5,5',6,6'-decanitrobiphenyl.
- 24-DNI*: C<sub>3</sub>H<sub>2</sub>N<sub>4</sub>O<sub>4</sub>; 2,4-dinitroimidazole.
- 14-DNI*: C<sub>3</sub>H<sub>2</sub>N<sub>4</sub>O<sub>4</sub>; 1,4-dinitroimidazole.
- EDNA*: C<sub>2</sub>H<sub>6</sub>N<sub>4</sub>O<sub>4</sub>; *N,N'*-Dinitro-1,2-ethenediamine
- HMX*: C<sub>4</sub>H<sub>8</sub>N<sub>8</sub>O<sub>8</sub>; octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine.
- HNB*: C<sub>6</sub>N<sub>6</sub>O<sub>12</sub>; hexanitrobenzene.
- HNS*: C<sub>14</sub>H<sub>6</sub>N<sub>6</sub>O<sub>12</sub>; 2,2',4,4',6,6'-hexanitrostilbene.
- HNBP*: C<sub>12</sub>H<sub>4</sub>N<sub>6</sub>O<sub>12</sub>; hexanitrobiphenyl.
- HNDDPM*: C<sub>13</sub>H<sub>6</sub>N<sub>6</sub>O<sub>12</sub>; 2,2',4,4',6,6'-hexanitrodiphenylmethane.
- Methyl picrate*: C<sub>7</sub>H<sub>5</sub>N<sub>3</sub>O<sub>7</sub>; 2-methoxy-1,3,5-trinitrobenzene.
- (MeNO<sub>2</sub>N)-22*: C<sub>8</sub>H<sub>6</sub>N<sub>6</sub>O<sub>10</sub>; *N*-methyl-2-amino-*N*,3,4,5,6-pentanitrotoluene.
- (MeNO<sub>2</sub>N)-23*: C<sub>8</sub>H<sub>6</sub>N<sub>6</sub>O<sub>10</sub>; *N*-methyl-3-amino-*N*,2,4,5,6-pentanitrotoluene.
- PNA*: C<sub>6</sub>H<sub>2</sub>N<sub>6</sub>O<sub>10</sub>; pentanitroaniline.
- PNB*: C<sub>6</sub>H<sub>5</sub>N<sub>5</sub>O<sub>10</sub>; pentanitrobenzene.
- PNT*: C<sub>7</sub>H<sub>3</sub>N<sub>5</sub>O<sub>10</sub>; pentanitrotoluene.
- Picric acid*: C<sub>6</sub>H<sub>3</sub>N<sub>3</sub>O<sub>7</sub>; 2,4,6-trinitrophenol.
- RDX*: C<sub>3</sub>H<sub>6</sub>N<sub>6</sub>O<sub>6</sub>; hexahydro-1,3,5-trinitrotriazine.
- Picryl azide*: C<sub>6</sub>H<sub>2</sub>N<sub>6</sub>O<sub>6</sub>; 2-azido-1,3,5-trinitrobenzene.
- PETN*: C<sub>5</sub>H<sub>8</sub>N<sub>4</sub>O<sub>12</sub>; tetranitrate pentaerythritol.
- tri245*: C<sub>3</sub>H<sub>5</sub>N<sub>5</sub>O<sub>6</sub>; 2,4,5-trinitroimidazole.
- TetNB*: C<sub>6</sub>H<sub>2</sub>N<sub>4</sub>O<sub>8</sub>; 1,2,3,5-tetranitrobenzene.
- TNB*: C<sub>6</sub>H<sub>3</sub>N<sub>3</sub>O<sub>6</sub>; 1,3,5-trinitrobenzene.
- TetNA*: C<sub>6</sub>H<sub>3</sub>N<sub>5</sub>O<sub>8</sub>; 2,3,4,6-tetranitroaniline.
- TNA*: C<sub>6</sub>H<sub>4</sub>N<sub>4</sub>O<sub>6</sub>; 2,4,6-trinitroaniline.
- TATB*: C<sub>6</sub>H<sub>6</sub>N<sub>6</sub>O<sub>6</sub>; 1,3,5-triamino-2,4,6-trinitrobenzene.
- 2,3,4,5-TetNT*: C<sub>7</sub>H<sub>4</sub>N<sub>4</sub>O<sub>8</sub>; 2,3,4,5-tetranitrotoluene.
- 2,3,4,6-TetNT*: C<sub>7</sub>H<sub>4</sub>N<sub>4</sub>O<sub>8</sub>; 2,3,4,6-tetranitrotoluene.
- 2,3,5,6-TetNT*: C<sub>7</sub>H<sub>4</sub>N<sub>4</sub>O<sub>8</sub>; 2,3,5,6-tetranitrotoluene.
- 2,4,6-TNT*: C<sub>7</sub>H<sub>5</sub>N<sub>3</sub>O<sub>6</sub>; 2,4,6-trinitrotoluene.
- 2,3,4-TNT*: C<sub>7</sub>H<sub>5</sub>N<sub>3</sub>O<sub>6</sub>; 2,3,4-trinitrotoluene.
- 3,4,5-TNT*: C<sub>7</sub>H<sub>5</sub>N<sub>3</sub>O<sub>6</sub>; 3,4,5-trinitrotoluene.
- TetN-o-Tol*: C<sub>7</sub>H<sub>5</sub>N<sub>5</sub>O<sub>8</sub>; 2-amino-3,4,5,6-tetranitrotoluene.
- TetN-m-Tol*: C<sub>7</sub>H<sub>5</sub>N<sub>5</sub>O<sub>8</sub>; 3-amino-2,4,5,6-tetranitrotoluene.
- TetN-p-Tol*: C<sub>7</sub>H<sub>5</sub>N<sub>5</sub>O<sub>8</sub>; 4-amino-2,3,5,6-tetranitrotoluene.
- Tetryl*: C<sub>7</sub>H<sub>5</sub>N<sub>5</sub>O<sub>8</sub>; *N*-methyl-*N*,2,4,6-tetranitroaniline.