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New Correlations for Predicting Impact Sensitivities of Nitro Energetic Compounds

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Some new and simple correlations have been introduced to predict impact sensitivities of various nitro energetic compounds. The correlations are based on the atomic numbers of C, H, N, O, and other amending factors, which are determined by the effect of the connective positions of groups to impact sensitivity. The predicted impact sensitivities for 196 energetic compounds are compared with the latest empirical computations presented by Keshavarz. Root mean square (rms) of deviation from experimental data is 37 cm, which is lower than that obtained from Keshavarz's computation (44 cm) [25,26].

Keywords: connective positions of groups, correlations, impact sensitivity, nitro energetic compounds

Introduction

Impact sensitivity is an important property for energetic materials. A large number of energetic materials cannot be used due to their high impact sensitivities. Impact sensitivity can be tested by experimental methods at the cost of consuming a

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large amount of samples. Therefore, predicting impact sensitivity theoretically is desirable. Extensive efforts have been made to predict the impact sensitivity of energetic compounds by quantum chemistry methods (or quantum mechanics computations) [1–18] and neural networks [19–21]. Each method is applicable to various nitro energetic compounds but requires either computational software or large numbers of data for a training set. To simplify the procedure, several correlations have been developed based on molecular structures. Kamlet [22,23] and Kamlet and Adolph [24] introduced an approach to classify the sensitivity of C–H–N–O explosives based on oxygen balance. Keshavarz and Pouretedal [25] and Keshavarz et al. [26] presented some better empirical correlations (see Eqs. (1a)–(1c)) for predicting impact sensitivity of a variety of nitro-derivated molecules recently, where a, b, c, and d are stoichiometric coefficients for an explosive of general formula $C_aH_bN_cO_d$ and MW is the molecular weight of the explosive. However, unfortunately, these methods did not take into account the effect of the connective positions of groups to impact sensitivities. For example, the experimental H_{50} of 2,4,6-trinitrotoluene, 2,3,4-trinitrotoluene, and 3,4,5-trinitrotoluene are 98, 56, and 107 cm [27], respectively. However, the predicted values of the above compounds are the same when calculated by both Kamlet's and Keshavarz's empirical correlations.

a. Polynitroaromatics (and benzofuroxans):

$$\log H_{50} = \frac{11.76a + 61.72b + 26.89c + 11.48d}{MW} \quad (1a)$$

b. Polynitroaromatics with α-CH and α-N-CH and nitramines:

$$\log H_{50} = \frac{47.33a + 23.50b + 2.357c - 1.105d}{MW} \quad (1b)$$

c. Polynitroaliphatics:

$$\log H_{50} = \frac{81.40a + 16.11b - 19.08c + 1.089d}{MW} \quad (1c)$$

In this study, we present some new and simple correlations for predicting impact sensitivities of nitro energetic compounds. The correlations will introduce some new factors to amend the effect of the connective positions of groups to impact sensitivities.

Because experimental data of impact sensitivity varied widely depending on testing machines, sample sizes, configurations, etc., we must consider the quality of experimental data to be used in establishing correlations. Therefore, experimental values of impact sensitivity were collected from Naval Surface Warfare Center (NSWC) [22–24,27–29] and the Los Alamos National Laboratory (LANL; J. R. Stine, personal communication, 1989), where the impact machines with the type 12 tool, 2.5 kg drop weight, and 25 trials were used. Many research works have demonstrated that the collected data are suitable for this work [1,19,20,25,30].

Details of the Correlations

Various $C_aH_bN_cO_d$ nitro energetic compounds have been studied, including nitroaromatics, nitroaliphatics, nitramines, and nitrate esters. It has been shown that the atomic numbers of C, H, N, O, and the amending factors play a role in determining the impact sensitivities. The following general equations are suitable for this purpose.

$$\log H_{50} = Aa' + Bb' + Cc' + Dd' + E + F \tag{2}$$

$$F = \sum Nn' \tag{3}$$

where F represents the amending factors that indicate the effect of the connective positions of groups to impact sensitivities. a', b', c', d', and n' are ratios of the atomic numbers of C, H, N, O, and groups with different connections to the molecular weight of $C_aH_bN_cO_d$ energetic compounds, respectively. A, B, C, D, E, and N are the accommodation coefficients, which amend the correlations to best fit the experimental data for different types of compounds. The detailed correlations to various energetic

compounds are as follows:

a. Polynitroaromatics (and benzofuroxans):

$$\log H_{50} = 19.86a' + 32.56b' - 12.71c' - 13.32d' + 1.68 + F1 \quad (4a)$$

b. Polynitroaromatics with α-CH and α-N-CH:

$$\log H_{50} = 22.48a' + 17.37b' - 31.40c' - 48.87d' + 2.62 + F2 \quad (4b)$$

c. Polynitroaliphatics:

$$\log H_{50} = 42.40a' + 16.30b' - 40.84c' - 31.53d' + 2.31 + F3 \quad (4c)$$

d. Nitroamines or nitrate esters:

$$\log H_{50} = 42.82a' + 12.46b' - 14.86c' - 21.47d' + 1.43 + F4 \quad (4d)$$

These divisions are similar to Keshavarz and Pouretedal's classifications [25]. The amending factors of $F1$, $F2$, $F3$, and $F4$ are presented in Tables 1–4, respectively.

Table 1
The amending factors of polynitroaromatics (and benzofuroxans)

	N		
Groups	$-NO_2$	$-NH_2$	$-OH$
Nitro	-*o* −7.90	-*o* 9.85	-*o* −2.64
	-*m* −20.28	-*m* 15.99	-*m* −33.39
	-*p* −7.46	-*p* 16.65	-*p* 1.98
Amino	-*o* 9.85	-*o* —	-*o* —
	-*m* 15.99	-*m* 14.72	-*m* —
	-*p* 16.65	-*p* —	-*p* —
Furoxan		1.81	

-*o*, -*m*, -*p* are ortho, meta, and para positions, respectively.

Table 2
The amending factors of polynitroaromatics with α-CH and α-N-CH

	N			
Groups	$-NO_2$	$-NH_2$	$-OH$	α-CH or α-N-CH
Nitro	-*o* −5.26	-*o* 15.31	-*o* 15.26	-*o* −6.69
	-*m* 1.92	-*m* 15.96	-*m* —	-*m* −0.69
	-*p* −11.36	-*p* 15.37	-*p* 30.53	-*p* −13.98
Amino	-*o* 15.31	-*o* —	-*o* —	-*o* —
	-*m* 15.96	-*m* —	-*m* —	-*m* —
	-*p* 15.37	-*p* —	-*p* —	-*p* —

-*o*, -*m*, -*p* are ortho, meta, and para positions, respectively.

Table 3
The amending factors of polynitroaliphatics

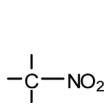
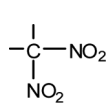
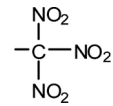
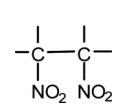
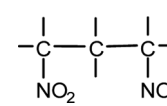
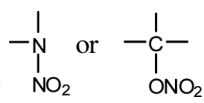
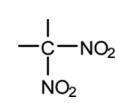
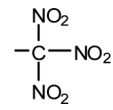
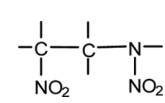
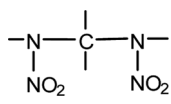
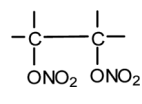
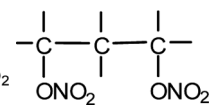
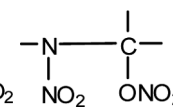
Groups					
N	−6.15	4.55	−32.75	−89.14	−56.50

Table 4
The amending factors of nitroamines or nitrate esters

Groups				
N	4.52	−4.20	−38.03	−28.19
				
N	6.96	7.15	−26.20	−57.53

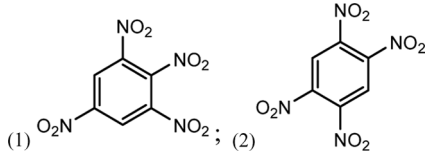
Details of the Prediction

The impact sensitivities of 196 nitro energetic compounds are predicted by Eqs. (4a)–(4d). The predicted results are compared with the ones obtained from Keshavarz's empirical correlations [25,26]. The root mean squares (rms) of deviation from experimental data are 37 and 44 cm, respectively. All results are shown in Table 5. Some examples of the details for predictions are shown below, and the results for each category are presented in Figs. 1(a)–(d). The results contain 52 polynitroaromatics (and benzofuroxans), 28 polynitroaromatics with α-CH and α-N-CH, 48 polynitroaliphatics, and 68 nitroamines or nitrate esters. The rms of the deviations are 45, 33, 33, and 34 cm (our results) and 56, 36, 43, and 35 cm (Keshavarz's results), respectively. Our results show better agreement with experimental values [27,30] compared to Keshavarz's results as a whole, but there are still some exceptions. The possible reason for the exceptions could be that the accommodation coefficients of the correlations are not accurate for some compounds. Therefore, more studies should be done to make this approach more credible.

Examples:

(a) Polynitroaromatics (and benzofuroxans):

- Compounds: $C_6H_2N_4O_8$
- Molecular weight: 258
- Structural formulae:



- Numbers of atoms: a = 6, b = 2, c = 4, d = 8
- Amending factors are (1) $n_{(NO2\text{-}o\text{-}NO2)} = 2$, $n_{(NO2\text{-}m\text{-}NO2)} = 3$, $n_{(NO2\text{-}p\text{-}NO2)} = 1$; (2) $n_{(NO2\text{-}o\text{-}NO2)} = 2$, $n_{(NO2\text{-}m\text{-}NO2)} = 2$, $n_{(NO2\text{-}p\text{-}NO2)} = 2$

Table 5

Experimental H_{50} and predicted values of new correlations, Keshavarz and Pouretedal [25] and Keshavarz et al. [26] for 196 nitro compounds

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
1	Hexanitrobenzene	$C_6N_6O_{12}^{(a)}$	11	6 (5)	12 (−1)
2	Pentanitrobenzene	$C_6HN_5O_{10}^{(a)}$	11	13 (−2)	18 (−7)
3	1,2,3,5-Tetranitrobenzene	$C_6H_2N_4O_8^{(a)}$	28	29 (−1)	34 (−6)
4	1,3,5-Trinitrobenzene	$C_6H_3N_3O_6^{(a)}$	71	72 (−1)	80 (−9)
5	2,4,6-Trinitrophenol	$C_6H_3N_3O_7^{(a)}$	64	59 (5)	66 (−2)
6	Pentanitroaniline	$C_6H_2N_6O_{10}^{(a)}$	22	26 (−4)	30 (−8)
7	2,3,4,6-Tetranitroaniline	$C_6H_3N_5O_8^{(a)}$	47	54 (−7)	59 (−12)
8	2,4,6-Trinitroaniline	$C_6H_4N_4O_6^{(a)}$	141	123 (18)	147 (−6)
9	1,3-Diamino-2,4,6-trinitrobenzene	$C_6H_5N_5O_6^{(a)}$	320	227 (93)	250 (70)
10	1,3,5-Triamino-2,4,6-trinitrobenzene	$C_6H_6N_6O_6^{(a)}$	490	446 (44)	401 (89)

(*Continued*)

Table 5

Continued

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
11	Hexanitrobiphenyl	$C_{12}H_4N_6O_{12}^{(a)}$	70	50 (20)	42 (28)
12	3,3′-Diamino-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{12}H_6N_8O_{12}^{(a)}$	67	89 (−22)	80 (−13)
13	4,4′-Diamino-2,2′,3,3′,5,5′,6,6′-octanitrobiphenyl	$C_{12}H_4N_{10}O_{16}^{(a)}$	57	45 (12)	35 (22)
14	4,6-Dinitrobenzofuroxan	$C_6H_2N_4O_6^{(a)}$	76	68 (8)	44 (32)
15	7-Amino-4,6-dinitrobenzofuroxan	$C_6H_3N_5O_6^{(a)}$	100	104 (−4)	81 (19)
16	5,7-Diamino-4,6-dinitrobenzofuroxan	$C_6H_4N_6O_6^{(a)}$	120	161 (−41)	138 (−18)
17	7-Amino-4,5,6-trinitrobenzofuroxan	$C_6H_2N_6O_8^{(a)}$	56	51 (5)	37 (19)
18	Benzotrifuroxan	$C_6N_6O_6^{(a)}$	53	36 (17)	16 (37)
19	Pentanitrotoluene	$C_7H_3N_5O_{10}^{(b)}$	18	11 (7)	19 (−1)
20	2,3,4,5-Tetranitrotoluene	$C_7H_4N_4O_8^{(b)}$	15	24 (−9)	37 (−22)

21	2,3,4,6-Tetranitrotoluene	$C_7H_4N_4O_8^{(b)}$	19	25 (−6)	37 (−18)
22	2,3,5,6-Tetranitrotoluene	$C_7H_4N_4O_8^{(b)}$	25	25 (0)	37 (−12)
23	2,4,6-Trinitrotoluene	$C_7H_5N_3O_6^{(b)}$	98	78 (20)	95 (3)
24	2,3,4-Trinitrotoluene	$C_7H_5N_3O_6^{(b)}$	56	72 (−16)	95 (−39)
25	3,4,5-Trinitrotoluene	$C_7H_5N_3O_6^{(b)}$	107	76 (31)	95 (12)
26	2-Amino-3,4,5,6-tetranitrotoluene	$C_7H_5N_5O_8^{(b)}$	36	42 (−6)	37 (−1)
27	3-Amino-2,4,5,6-tetranitrotoluene	$C_7H_5N_5O_8^{(b)}$	37	42 (−5)	37 (0)
28	4-Amino-2,3,5,6-tetranitrotoluene	$C_7H_5N_5O_8^{(b)}$	47	42 (5)	37 (10)
29	2,2′,4,4′,6,6′-Hexanitrodiphenylmethane	$C_{13}H_6N_6O_{12}^{(b)}$	39	45 (−6)	53 (−14)
30	2-Azido-1,3,5-trinitrobenzene	$C_6H_2N_6O_6^{(a)}$	19	35 (−16)	47 (−28)
31	Azidopentanitrobenzene	$C_6N_8O_{10}^{(a)}$	17	9 (8)	15 (2)
32	N-Methyl-N,2,4,6-tetranitroaniline	$C_7H_5N_5O_8^{(b)}$	25	31 (−6)	37 (−12)
33	N-Methyl-2-amino-N,3,4,5,6-pentanitrotoluene	$C_8H_6N_6O_{10}^{(b)}$	21	20 (1)	32 (−11)
34	N-Methyl-3-amino-N,2,4,5,6-pentanitrotoluene	$C_8H_6N_6O_{10}^{(b)}$	18	19 (−1)	32 (−14)
35	1,2,4,5-Tetranitrobenzene	$C_6H_2N_4O_8^{(a)}$	27	32 (−5)	34 (−7)

(*Continued*)

Table 5

Continued

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
36	2,4,6-Trinitroresorcinol	$C_6H_3N_3O_8^{(a)}$	43	50 (−7)	56 (−13)
37	2,4,6-Trinitrophloro-glucinol	$C_6H_3N_3O_9^{(a)}$	27	43 (−16)	49 (−22)
38	2,4-Dinitroresorcinol	$C_6H_4N_2O_6^{(a)}$	296	185 (111)	159 (137)
39	4,6-Dinitroresorcinol	$C_6H_4N_2O_6^{(a)}$	320	195 (125)	159 (161)
40	2,4,6-Trinitro-3-aminophenol	$C_6H_4N_4O_7^{(a)}$	138	99 (39)	118 (20)
41	1,3-Diamino-2,4,6-trinitrobenzene	$C_6H_5N_5O_6^{(a)}$	320	227 (93)	250 (70)
42	1-Hydroxyl-3,5-diamino-2,4,6-trinitrobenzene	$C_6H_5N_5O_7^{(a)}$	120	178 (−58)	197 (−77)
43	Ammonium picrate	$C_6H_6N_4O_7^{(a)}$	135	133 (2)	361 (−226)
44	2,4,6-Trinitrobenzonitrile	$C_7H_2N_4O_6^{(a)}$	140	54 (86)	41 (99)
45	2,4,6-Trinitrobenzoic acid	$C_7H_3N_3O_8^{(a)}$	109	63 (46)	52 (57)
46	2,4,6-Trinitroanisole	$C_7H_5N_3O_7^{(a)}$	192	134 (58)	188 (4)
47	3-Methoxy-2,4,6-trinitroaniline	$C_7H_6N_4O_7^{(a)}$	320	209 (111)	305 (15)

48	1,3-Dimethoxy-2,4,6-trinitrobenzene	$C_8H_7N_3O_8^{(a)}$	251	219 (32)	364 (−113)
49	2′,2′,2′-Trinitroethyl-2,4,6-trinitrobenzoate	$C_9H_4N_6O_{14}^{(a)}$	24	44 (−20)	41 (−17)
50	2′,2′,2′-Trinitroethyl-3,5-dinitrobenzoate	$C_9H_5N_5O_{12}^{(a)}$	73	87 (−14)	68 (5)
51	2′,2′,2′-Trinitroethyl-3,5-dinitrosalicylate	$C_9H_5N_5O_{13}^{(a)}$	45	53 (−8)	61 (−16)
52	1,4,5,8-Tetranitro-napthalene	$C_{10}H_4N_4O_8^{(a)}$	100	153 (−53)	68 (32)
53	2′,2′-Dinitropropyl-2,4,6-trinitrobenzoate	$C_{10}H_7N_5O_{12}^{(a)}$	214	110 (104)	130 (84)
54	2,2′,4,4′,6,6′-Hexanitrobiphenyl	$C_{12}H_4N_6O_{12}^{(a)}$	85	50 (35)	42 (43)
55	3-Hydroxy-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{12}H_4N_6O_{13}^{(a)}$	42	46 (−4)	39 (3)
56	3,3′-Dihydroxy-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{12}H_4N_6O_{14}^{(a)}$	40	42 (−2)	36 (4)
57	2,2′,4,4′,6,6′-Hexanitro-biphenylamine	$C_{12}H_5N_7O_{12}^{(a)}$	48	82 (−34)	59 (−11)
58	3,3′-Diamino-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{12}H_6N_8O_{12}^{(a)}$	132	89 (43)	80 (52)

(*Continued*)

Table 5

Continued

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
59	2,2′,4,4′,6-Pentanitro-benzophenone	$C_{13}H_5N_5O_{11}^{(a)}$	54	99 (−45)	60 (−6)
60	2,2′,2″,4,4′,4″,6,6′6″-Nonanitro-m-terphenyl	$C_{18}H_5N_9O_{18}^{(a)}$	39	45 (−6)	34 (5)
61	2, 2″,4,4′,4″,6,6′6″-Octanitro-m-terphenyl	$C_{18}H_6N_8O_{16}^{(a)}$	63	69 (−6)	46 (17)
62	2, 2′,2″,4,4″,5′,6,6″-Octanitro-p-terphenyl	$C_{18}H_6N_8O_{16}^{(a)}$	40	73 (−33)	46 (−6)
63	2, 2′,2″,4,4″,6,6′,6″-Octanitro-p-terphenyl	$C_{18}H_6N_8O_{16}^{(a)}$	59	69 (−10)	46 (13)
64	Dodecanitroquaterphenyl	$C_{24}H_6N_{12}O_{24}^{(a)}$	40	42 (−2)	30 (10)
65	2.4.6-Trinitrobenzaldehyde	$C_7H_3N_3O_7^{(a)}$	36	73 (−37)	60 (−24)
66	2,4,6-Trinitrobenzaldoxime	$C_7H_4N_4O_7^{(a)}$	42	85 (−43)	105 (−63)
67	1-Dinitromethyl-3-nitrobenzene	$C_7H_5N_3O_6^{(b)}$	105	97 (8)	95 (10)
68	2,4,6-Trinitrobenzylalcohol	$C_7H_5N_3O_7^{(b)}$	52	55 (−3)	70 (−18)

69	2,4,6-Trinitro-m-cresol	$C_7H_5N_3O_7^{(b)}$	191	98 (93)	70 (121)
70	1-(2,2,2-Trinitroethyl)-2,4,6-trinitrobenzene	$C_8H_4N_6O_{12}^{(b)}$	13	15 (−2)	18 (−5)
71	2,4,6-Trinitrostyrene	$C_8H_5N_3O_6^{(b)}$	32	106 (−74)	119 (−87)
72	1-(2,2,2-Trinitroethyl)-2,4-dinitrobenzene	$C_8H_5N_5O_{10}^{(b)}$	31	26 (5)	32 (−1)
73	3,5-Dimethyl-2,4,6-trinitrophenol	$C_8H_7N_3O_7^{(b)}$	77	139 (−62)	129 (−52)
74	1-(3,3,3-Trinitropropyl)-2,4,6-trinitrobenzene	$C_9H_6N_6O_{12}^{(b)}$	21	23 (−2)	29 (−8)
75	1-(3,3,3-Trinitropropyl)-2,4-dinitrobenzene	$C_9H_7N_5O_{10}^{(b)}$	31	43 (−12)	52 (−21)
76	3-Methyl-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{13}H_6N_6O_{12}^{(b)}$	53	52 (1)	53 (0)
77	3-Methyl-2,2′,4,4′,6-pentanitrobiphenyl	$C_{13}H_7N_5O_{10}^{(b)}$	143	95 (48)	97 (46)
78	Hexanitrostilbene	$C_{14}H_6N_6O_{12}^{(b)}$	39	54 (−15)	61 (−22)
79	2,2′,4,4′,6,6′-Hexanitrobibenzyl	$C_{14}H_8N_6O_{12}^{(b)}$	114	65 (49)	76 (38)
80	3,3′-Dimethyl-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{14}H_8N_6O_{12}^{(b)}$	135	65 (70)	76 (59)

(*Continued*)

Table 5

Continued

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
81	1,1,1,3-Tetranitrobutane	$C_4H_6N_4O_8^{(c)}$	33	19 (14)	31 (2)
82	1,1,1,3,5,5,5-Heptanitropentene	$C_5H_5N_7O_{14}^{(c)}$	8	5 (3)	9 (−1)
83	1,1,1,6,6,6-Hexanitro-3-hexyne	$C_6H_4N_6O_{12}^{(c)}$	7	18 (−11)	19 (−12)
84	1,1,1,6,6,6-Hexanitro-3-hexene	$C_6H_6N_6O_{12}^{(c)}$	17	23 (−6)	23 (−6)
85	3,3,4,4-Tetranitrohexane	$C_6H_{10}N_4O_8^{(c)}$	80	104 (−24)	154 (−74)
86	2,2,4,4,6,6-Hexanitroheptane	$C_7H_{10}N_6O_{12}^{(c)}$	29	40 (−11)	50 (−21)
87	2,2,4,6,6-Pentanitroheptane	$C_7H_{11}N_5O_{10}^{(c)}$	56	69 (−13)	109 (−53)
88	2,2,2-Trinitroethylcarbamate	$C_3H_4N_4O_8^{(c)}$	18	15 (3)	12 (6)
89	2,2-Dinitro-1,3-propanediol	$C_3H_6N_2O_6^{(c)}$	110	116 (−6)	73 (37)
90	Methyl-2,2,2-trinitroethyl-carbonate	$C_4H_5N_3O_9^{(c)}$	28	34 (−6)	32 (−4)
91	4,4,4-Trinitrobutyramide	$C_4H_6N_4O_7^{(c)}$	40	44 (−4)	39 (1)
92	Bis-(2,2,2-trinitroethyl)-carbonate	$C_5H_4N_6O_{15}^{(c)}$	16	10 (6)	9 (7)

93	Methylene-bis-N,N′-(2,2,2-trinitroacetamide)	$C_5H_4N_8O_{14}^{(c)}$	9	8 (1)	7 (2)
94	Bis-(trinitroethoxy)-methane	$C_5H_6N_6O_{14}^{(c)}$	17	13 (4)	12 (5)
95	N,N′-Bis-(2,2,2-trinitroethyl)-urea	$C_5H_6N_8O_{13}^{(c)}$	17	11 (6)	9 (8)
96	5,5,5-Trinitropentanone-2	$C_5H_7N_3O_7^{(c)}$	125	122 (3)	134 (−9)
97	Ethyl-2,2,2-trinitroethyl carbonatesize	$C_5H_7N_3O_9^{(c)}$	81	73 (8)	74 (7)
98	N-(2-Propyl)-trinitroacetamide	$C_5H_8N_4O_7^{(c)}$	112	99 (13)	95 (17)
99	Bis-(trinitroethyl)-oxalate	$C_6H_4N_6O_{16}^{(c)}$	15	13 (2)	12 (3)
100	2,2,2-Trinitroethyl-4,4,4-trinitrobutrate	$C_6H_6N_6O_{14}^{(c)}$	18	19 (−1)	18 (0)
101	Bis-(trinitroethyl)-oxamide	$C_6H_6N_8O_{14}^{(c)}$	13	14 (−1)	12 (1)
102	Trinitroethyl-2,2-dinitropropylcarbonate	$C_6H_7N_5O_{13}^{(c)}$	15	35 (−20)	29 (−14)
103	N-Trinitroethyl-4,4,4-trinitrobutramide	$C_6H_7N_7O_{13}^{(c)}$	18	20 (−2)	18 (0)
104	1,5-Bis-(trinitroethyl)-biuret	$C_6H_7N_9O_{14}^{(c)}$	24	14 (10)	11 (13)
105	N(t-Butyl)-trinitroacetamide	$C_6H_{10}N_4O_7^{(c)}$	110	206 (−96)	210 (−100)

(*Continued*)

Table 5

Continued

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
106	1,1,1,7,7,7-Hexanitroheptanone-4	$C_7H_8N_6O_{13}^{(c)}$	34	35 (−1)	36 (−2)
107	2,2-Dinitropropyltrinitrobutyrate	$C_7H_9N_5O_{12}^{(c)}$	151	69 (82)	60 (91)
108	2,2,2-Trinitroethyl-4,4-dinitrovalerate	$C_7H_9N_5O_{12}^{(c)}$	70	69 (1)	60 (10)
109	Bis-(2,2-dinitropropyl)-carbonate	$C_7H_{10}N_4O_{11}^{(c)}$	300	153 (147)	111 (189)
110	2,2-Dinitropropyl-4,4,4-trinitrobutyramide	$C_7H_{10}N_6O_{11}^{(c)}$	72	72 (0)	60 (12)
111	Bis-(trinitropropyl)-urea	$C_7H_{10}N_8O_{13}^{(c)}$	23	31 (−8)	27 (−4)
112	Bis-(1,1,1-trinitro-2-propy)-urea	$C_7H_{10}N_8O_{13}^{(c)}$	19	31 (−12)	27 (−8)
113	Bis-(trinitroethyl)-fumarate	$C_8H_6N_6O_{16}^{(c)}$	14	29 (−15)	30 (−16)
114	Trinitroethyl-bis-(trinitroethoxy)-acetate	$C_8H_7N_9O_{22}^{(c)}$	6	12 (−6)	11 (−5)
115	4,4,4-Trinitrobutyric anhydride	$C_8H_8N_6O_{15}^{(c)}$	30	38 (−8)	39 (−9)
116	Bis-(2,2,2-trinitroethyl)-succinate	$C_8H_8N_6O_{16}^{(c)}$	30	34 (−4)	35 (−5)

117	Bis-(2,2-dinitropropyl)-oxalate	$C_8H_{10}N_4O_{12}^{(c)}$	227	168 (59)	131 (96)
118	N,N′-Bis-(3,3,3-trinitropropyl)-oxamide	$C_8H_{10}N_8O_{14}^{(c)}$	45	36 (9)	34 (11)
119	2,2,2-Trinitroethyl-4,4-dinitrohexanoate	$C_8H_{11}N_5O_{12}^{(c)}$	138	115 (23)	105 (33)
120	2,2-Dinitrobutyl-4,4,4-trinitrobutramide	$C_8H_{11}N_5O_{12}^{(c)}$	101	115 (−14)	105 (−4)
121	2,2-Dinitropropyl-4,4-dinitrovalerate	$C_8H_{12}N_4O_{10}^{(c)}$	320	326 (−6)	254 (66)
122	Nitroisobutyl-4,4,4-trinitrobutrate	$C_8H_{12}N_4O_{10}^{(c)}$	279	232 (47)	254 (25)
123	Methylene-bis-(4,4,4-trinitrobutramide)	$C_9H_{12}N_8O_{14}^{(c)}$	113	56 (57)	54 (59)
124	Ethylene-bis-(4,4,4-trinitrobutrate)	$C_{10}H_{12}N_6O_{16}^{(c)}$	120	79 (41)	85 (35)
125	N,N-Bis-(2,2-dinitropropyl)-4,4,4-trinitrobutramide	$C_{10}H_{14}N_8O_{15}^{(c)}$	72	91 (−19)	72 (0)
126	Bis-(2,2,2-trinitroethyl)-4,4-dinitroheptanedioate	$C_{11}H_{12}N_8O_{20}^{(c)}$	68	49 (19)	46 (22)
127	2,2-Dinitropropane-1,3-diol-(4,4,4-trinitrobutrate)	$C_{11}H_{12}N_8O_{20}^{(c)}$	50	49 (1)	46 (4)

(*Continued*)

Table 5

Continued

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
128	Bis-(2,2,2-trinitroethyl)-4,4,6,6,8,8-hexanitro-undecanedioate	$C_{15}H_{16}N_{12}O_{28}^{(c)}$	32	33 (−1)	38 (−6)
129	N,N′-Dinitromethanediamine	$CH_4N_4O_4^{(d)}$	13	15 (−2)	12 (1)
130	N-Nitro-N-methyl-formamide	$C_2H_4N_2O_3^{(d)}$	320	75 (245)	67 (253)
131	N,N′-Dinitro-1,2-ethanediamine	$C_2H_6N_4O_4^{(d)}$	34	39 (−5)	40 (−6)
132	Methyl-2,2,2-trinitroethyl-nitramine	$C_3H_5N_5O_8^{(d)}$	9	9 (0)	13 (−4)
133	Trinitroethylnitrguanidine	$C_3H_5N_7O_8^{(d)}$	15	10 (5)	10 (5)
134	Cyclotrimethylenetrinitramine	$C_3H_6N_6O_6^{(d)}$	26	27 (−1)	20 (6)
135	N-Methyl-N,N′-dinitro-1,2,3-ethanediamine	$C_3H_8N_4O_4^{(d)}$	114	99 (15)	110 (4)
136	Trinitroethylcyanomethyl-nitramine	$C_4H_4N_6O_8^{(d)}$	11	11 (0)	12 (−1)

137	Bis-(2,2,2-trinitroethyl)-nitramine	$C_4H_4N_8O_{14}^{(d)}$	5	4 (1)	5 (0)
138	N-Methyl-N-nitro-(trinitroethyl)-carbamate	$C_4H_5N_5O_{10}^{(d)}$	17	13 (4)	12 (5)
139	N,N′-Dimethyl-N,N′-dinitrooxamide	$C_4H_6N_4O_6^{(d)}$	79	57 (22)	41 (38)
140	N-Nitro-N(trinitroethyl)-glycinamide	$C_4H_6N_6O_9^{(d)}$	17	12 (5)	15 (2)
141	Cyclotetramethylenetetranitramine	$C_4H_8N_8O_8^{(d)}$	29	27 (2)	20 (9)
142	N,N′-Dinitro-N-[2-(nitroamino) ethyl]-1,2-ethanediamine	$C_4H_{10}N_6O_6^{(d)}$	39	66 (−27)	65 (−26)
143	1,3,3,5,5-Pentanitro piperidine	$C_5H_6N_6O_{10}^{(d)}$	14	16 (−2)	17 (−3)
144	2,2,2-Trinitroethyl-3′,3′,3′-trinitropropylnitramine	$C_5H_6N_8O_{14}^{(d)}$	6	7 (−1)	9 (−3)
145	N,N′-Bis-2,2,2-trinitroethyl-N,N′-dinitromethanediamine	$C_5H_6N_{10}O_{16}^{(d)}$	5	6 (−1)	7 (−2)
146	Trinitroethyl-N-ethyl-N-nitro-carbamate	$C_5H_7N_5O_{10}^{(d)}$	19	23 (−4)	23 (−4)
147	Trinitroethyl-2-methoxy-ethylnitramine	$C_5H_9N_5O_9^{(d)}$	42	27 (15)	39 (3)

(*Continued*)

Table 5

Continued

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
148	N-Methyl-N′-trinitroethyl-N,N′-dinitro-1,2-ethanediamine	$C_5H_9N_7O_{10}^{(d)}$	11	19 (−8)	24 (−13)
149	N,N′-3,3-tetranitro-1,5-pentanediamine	$C_5H_{10}N_6O_8^{(d)}$	35	53 (−18)	49 (−14)
150	N-Nitro-N-(3,3,3-trinitropropyl)-2,2,2-trinitroethyl carbamate	$C_6H_6N_8O_{16}^{(d)}$	9	10 (−1)	9 (0)
151	2,2,2-Trinitroethyl-N-(2,2,2-trinitroethyl)-nitramino acetate	$C_6H_6N_8O_{16}^{(d)}$	9	7 (2)	9 (0)
152	2,2,2-Trinitroethyl-4-nitrazavalerate	$C_6H_9N_5O_{10}^{(d)}$	35	38 (−3)	39 (−4)
153	Trinitropropyl-(2,2-dinitropropyl)-nitramine	$C_6H_9N_7O_{12}^{(d)}$	17	19 (−2)	22 (−5)
154	2′,2′,2′-Trinitroethyl-2,5-dinitrazahexanoate	$C_6H_9N_7O_{12}^{(d)}$	15	24 (−9)	22 (−7)

155	2,2,2-Trinitroethyl-3,3′-dinitrobuthyl nitramine	$C_6H_9N_7O_{12}^{(d)}$	20	19 (1)	22 (−2)
156	N-(2,2-Dinitropropyl)-N,2,2-trinitro-1-propanamine	$C_6H_{10}N_6O_{10}^{(d)}$	29	31 (−2)	40 (−11)
157	1,7-Dimethoxy-2,4,6-trinitrazaheptane	$C_6H_{14}N_6O_8^{(d)}$	166	125 (41)	119 (47)
158	N,N′-Dinitro-N,N′-bis[2-(nitroamino)ethyl]-1,2-ethanediamine	$C_6H_{14}N_8O_8^{(d)}$	53	83 (−30)	81 (−28)
159	Bis-(trinitroethyl)-2,4-dinitrazapentanedioate	$C_7H_6N_{10}O_{20}^{(d)}$	10	9 (1)	7 (3)
160	2,2-Dinitropropyl-5,5,5-trinitro-2-nitrazapentanoate	$C_7H_9N_7O_{14}^{(d)}$	16	23 (−7)	20 (−4)
161	Trinitroethyl-5,5-dinitro-3-nitrazahexanoate	$C_7H_9N_7O_{14}^{(d)}$	25	20 (5)	20 (5)
162	2,2,2-Trinitroethyl-2,5,5-trinitro-2-azahexanoate	$C_7H_9N_7O_{14}^{(d)}$	22	23 (−1)	20 (2)
163	N-Nitro-N,N′-bis(trinitropropyl)-urea	$C_7H_9N_9O_{15}^{(d)}$	21	15 (6)	16 (5)
164	2,2,2-Trinitroethyl-2,4,6,6-tetranitro-2,4-diazaheptanoate	$C_7H_9N_9O_{16}^{(d)}$	18	15 (3)	14 (4)

(*Continued*)

Table 5

Continued

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
165	Bis-(2,2,2-trinitroethyl)-3-nitrazaglutarate	$C_8H_8N_8O_{18}^{(d)}$	14	15 (−1)	13 (1)
166	N,N′-Dinitro-N,N′-bis-3,3,3-Trinitropropyl-oxamide	$C_8H_8N_{10}O_{18}^{(d)}$	9	14 (−5)	12 (−3)
167	Bis-(trinitroethyl)-2,4,6-trinitraza-heptanedioate	$C_8H_8N_{12}O_{22}^{(d)}$	13	11 (2)	8 (5)
168	2,2,6,9,9-Pentanitro-4-oxa-5-oxo-6-azadecane	$C_8H_{12}N_6O_{12}^{(d)}$	47	63 (−16)	53 (−6)
169	1,1,1,3,6,9,11,11,11-Nonanitro-3,6,9-triazaundecane	$C_8H_{12}N_{12}O_{18}^{(d)}$	12	12 (0)	15 (−3)
170	N-(2,2-Dinitrobutyl)-N-2,2-trinitro-1-butanamine	$C_8H_{14}N_6O_{10}^{(d)}$	80	73 (7)	102 (−22)
171	N,N′-Dinitro-N,N′-bis-(3-nitrazabutyl)-oxamide	$C_8H_{14}N_8O_{10}^{(d)}$	90	91 (−1)	75 (15)
172	2,2,4,7,9,9-Hexanitro-4,7-diazadecane	$C_8H_{14}N_8O_{12}^{(d)}$	72	43 (29)	53 (19)

173	N,N′-Dinitromethylene-bis-(4,4,4-trinitro)-butyramide	$C_9H_{10}N_{10}O_{18}^{(d)}$	13	19 (−6)	16 (−3)
174	1,1,1,5,710,14,14,14-Nonanitro-3,12-dioxa-4,11-dioxo-5,7,10-triazatetradecane	$C_9H_{10}N_{12}O_{22}^{(d)}$	11	13 (−2)	11 (0)
175	Bis-(5,5,5-trinitro-3-nitrazapentanoyl)-methylenedinitramine	$C_9H_{10}N_{14}O_{22}^{(d)}$	15	10 (5)	10 (5)
176	1,1,1,4,6,6,8,11,11,11-Decanitro-4,8-diazaundecane	$C_9H_{12}N_{12}O_{20}^{(d)}$	11	13 (−2)	15 (−4)
177	1,1,1,3,6,6,9,11,11,11-Decanitro-3,9-diazaundecane	$C_9H_{12}N_{12}O_{20}^{(d)}$	10	13 (−3)	15 (−5)
178	Bis-(2,2,2-trinitroethyl)-4-nitraza-1,7-heptanedioate	$C_{10}H_{12}N_8O_{18}^{(d)}$	29	27 (2)	26 (3)
179	Bis-(2,2,2-trinitroethyl)-3,6-dinitraza-1,8-octanedioate	$C_{10}H_{12}N_{10}O_{20}^{(d)}$	29	21 (8)	19 (10)
180	Bis-(trinitroethyl)-2,5,8-trinitraza nonanedioate	$C_{10}H_{12}N_{12}O_{22}^{(d)}$	17	17 (0)	15 (2)
181	N,N′-Dinitro-N,N′-bis-(3,3-dinitrobutyl)-oxamide-triazatetradecane	$C_{10}H_{14}N_8O_{14}^{(d)}$	37	30 (7)	52 (−15)

(*Continued*)

Table 5

Continued

No.	Compound names	Formula[a]	H_{50} (exp.)[b] (cm)	Our result[c] (cm)	Result by Keshavarz et al.[c] (cm)
182	1,1,1,3,6,9,12,14,14,14-Decanitro-, 6,9,12-tetrazatetradecane	$C_{10}H_{16}N_{14}O_{20}^{(d)}$	19	18 (1)	21 (−2)
183	Bis-(trinitroethyl)-5,5-dinitro-2,8-dinitraza-nonanedioate	$C_{11}H_{12}N_{12}O_{24}^{(d)}$	12	17 (−5)	14 (−2)
184	2,2,4,7,7,10,12,12-Octanitro-4, 10-diazatridecane	$C_{11}H_{18}N_{10}O_{16}^{(d)}$	44	50 (−6)	55 (−11)
185	2,2,5,7,7,9,12,12-Octanitro-5, 9-diazatridecane	$C_{11}H_{18}N_{10}O_{16}^{(d)}$	37	50 (−13)	55 (−18)
186	1,4-Bis-(5,5,5-trinitro-2-nitrazapentanoate)-2-butyne	$C_{12}H_{12}N_{10}O_{20}^{(d)}$	16	29 (−13)	24 (−8)
187	1,1,1,18,18,18-Hexanitro-3,16-dioxa-4,15-dioxo-5,8,11,14-tetranitrazaoctadecane	$C_{12}H_{16}N_{14}O_{24}^{(d)}$	19	22 (−3)	19 (0)
188	1,1,1,3,6,6,8,10,10,13,15,15,15-Tridecanitro-3,8,13-triazapentadecane	$C_{12}H_{16}N_{16}O_{26}^{(d)}$	23	13 (10)	16 (7)

189	2,2-Dinitropropanediol-bis-(5,5-dinitro-2-nitraza-hexanoate)	$C_{13}H_{18}N_{10}O_{20}^{(d)}$	138	56 (82)	44 (94)
190	1,2,3-Propanetriol trinitrate	$C_3H_5N_3O_9^{(d)}$	20	22 (−2)	17 (3)
191	N-(2,2,2-Trinitroethyl)-nitraminoethyl nitrate	$C_4H_6N_6O_{11}^{(d)}$	7	7 (0)	10 (−3)
192	2,2-Bis-(nitroxymethyl)-1,3-propanediol dinitrate	$C_5H_8N_4O_{12}^{(d)}$	13	14 (−1)	31 (−18)
193	3-[N-(2,2,2-Trinitroethyl)-nitramino]-propyl nitrate	$C_5H_8N_6O_{11}^{(d)}$	12	17 (−5)	21 (−9)
194	3,5,5-Trinitro-3-azahexyl nitrate	$C_5H_9N_5O_9^{(d)}$	21	36 (−15)	44 (−23)
195	1,9-Dinitrato-2,4,6,8-tetranitrazanonane	$C_5H_{10}N_{10}O_{14}^{(d)}$	10	11 (−1)	8 (2)
196	4,4,8,8-Tetranitro-1,11-dinitro-6-nitraza undecane	$C_{10}H_{16}N_8O_{16}^{(d)}$	87	46 (41)	72 (15)
rms Deviation (cm)				37	44

[a]The types of compounds are marked at the top right corner of formulae. (a) Polynitroaromatics (and benzofuroxans); (b) polynitroaromatics with a-CH and a-N-CH; (c) polynitroaromatics; (d) nitroamines or nitrate esters.

[b]Reported H_{50} values for numbers 1 to 34 were taken from Wilson et al. [27] and the other values from Storm et al. [30], and all of them were tested by drop weight impact tests with the type 12 tool, 2.5 kg drop weight, and 25 trials.

[c]Difference in H_{50} values (in cm) given in parentheses.

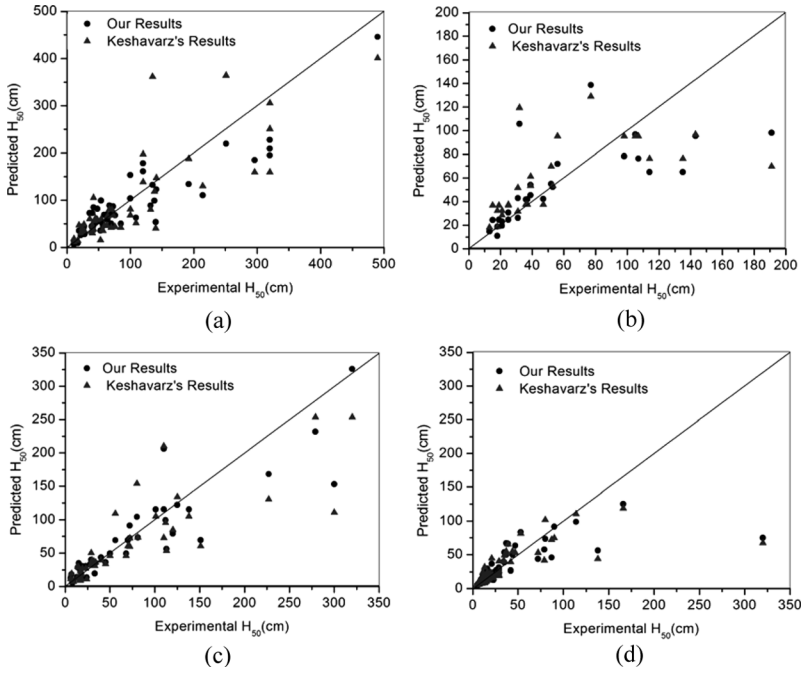


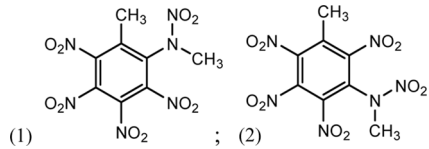
Figure 1. The predicted impact sensitivities of nitro compounds and their comparisons to experimental and Keshavarz's results. (a) Polynitroaromatics (and benzofuroxans); (b) polynitroaromatics with α-CH and α-N-CH; (c) polynitroaliphatics; (d) nitroamines or nitrate esters.

$$\begin{aligned}\log H_{50}(1) &= 19.86 \times \frac{6}{258} + 32.56 \times \frac{2}{258} - 12.71 \\ &\quad \times \frac{4}{258} - 13.32 \times \frac{8}{258} + 1.68 - 7.90 \\ &\quad \times \frac{2}{258} - 20.28 \times \frac{3}{258} - 7.46 \times \frac{1}{258} \\ &= 1.458\end{aligned}$$

$$\log H_{50}(2) = 19.86 \times \frac{6}{258} + 32.56 \times \frac{2}{258} - 12.71 \times \frac{4}{258} - 13.32 \times \frac{8}{258} + 1.68 - 7.90 \times \frac{2}{258} - 20.28 \times \frac{2}{258} - 7.46 \times \frac{2}{258} = 1.508$$

(b) Polynitroaromatics with α-CH and α-N-CH:

- Compounds: $C_8H_6N_6O_{10}$
- Molecular weight: 346
- Structural formulae:



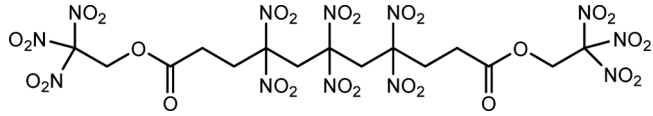
- Numbers of atoms: a = 8, b = 6, c = 6, d = 10
- Amending factors are (1) $n_{(\mathrm{NO2}\text{-}o\text{-}\mathrm{NO2})} = 3$, $n_{(\mathrm{NO2}\text{-}m\text{-}\mathrm{NO2})} = 2$, $n_{(\mathrm{NO2}\text{-}p\text{-}\mathrm{NO2})} = 1$, $n_{(\mathrm{NO2}\text{-}o\text{-}(\alpha\text{-CH or }\alpha\text{-N-CH}))} = 2$, $n_{(\mathrm{NO2}\text{-}m\text{-}(\alpha\text{-CH or }\alpha\text{-N-CH}))} = 2$, $n_{(\mathrm{NO2}\text{-}p\text{-}(\alpha\text{-CH or }\alpha\text{-N-CH}))} = 2$; (2) $n_{(\mathrm{NO2}\text{-}o\text{-}\mathrm{NO2})} = 2$, $n_{(\mathrm{NO2}\text{-}m\text{-}\mathrm{NO2})} = 3$, $n_{(\mathrm{NO2}\text{-}p\text{-}\mathrm{NO2})} = 1$, $n_{(\mathrm{NO2}\text{-}o\text{-}(\alpha\text{-CH or }\alpha\text{-N-CH}))} = 4$, $n_{(\mathrm{NO2}\text{-}m\text{-}(\alpha\text{-CH or }\alpha\text{-N-CH}))} = 2$, $n_{(\mathrm{NO2}\text{-}p\text{-}(\alpha\text{-CH or }\alpha\text{-N-CH}))} = 2$

$$\log H_{50}(1) = 22.48 \times \frac{8}{346} + 17.37 \times \frac{6}{346} - 31.40 \times \frac{6}{346} - 48.87 \times \frac{10}{346} + 2.62 - 5.26 \times \frac{3}{346} + 1.92 \times \frac{2}{346} - 11.36 \times \frac{1}{346} - 6.69 \times \frac{2}{346} - 0.69 \times \frac{2}{346} - 13.98 \times \frac{2}{346} = 1.294$$

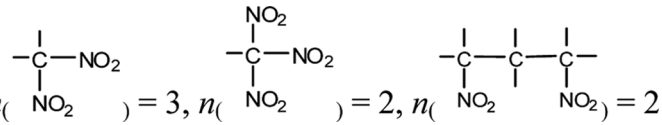
$$\begin{aligned}\log H_{50}(2) = 22.48 \times \frac{8}{346} + 17.37 \times \frac{6}{346} - 31.40 \times \frac{6}{346} \\ - 48.87 \times \frac{10}{346} + 2.62 - 5.26 \times \frac{2}{346} + 1.92 \\ \times \frac{3}{346} - 11.36 \times \frac{1}{346} - 6.69 \times \frac{4}{346} - 0.69 \\ \times \frac{2}{346} - 13.98 \times \frac{2}{346} \\ = 1.276\end{aligned}$$

(c) Polynitroaliphatics:

- Compound: $C_{15}H_{16}N_{12}O_{28}$
- Molecular weight: 812
- Structural formula:



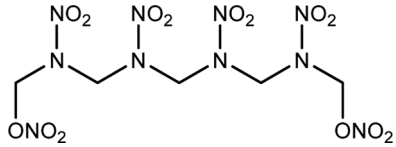
- Numbers of atoms: a = 15, b = 16, c = 12, d = 28
- Amending factors are



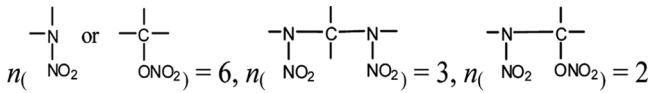
$$\begin{aligned}\log H_{50} = 42.40 \times \frac{15}{812} + 16.30 \times \frac{16}{812} - 40.84 \\ \times \frac{12}{812} - 31.53 \times \frac{28}{812} + 2.31 + 4.55 \\ \times \frac{3}{812} - 32.75 \times \frac{2}{812} - 56.50 \times \frac{2}{812} \\ = 1.522\end{aligned}$$

(d) Nitroamines or nitrate esters:

- Compound: $C_5H_{10}N_{10}O_{14}$
- Molecular weight: 434
- Structural formula:



- Numbers of atoms: a = 5, b = 10, c = 10, d = 14
- Amending factors are



$$\log H_{50} = 42.82 \times \frac{5}{434} + 12.46 \times \frac{10}{434} - 14.86 \times \frac{10}{434} - 21.47 \times \frac{14}{434} + 1.43 + 4.52 \times \frac{6}{434} + 6.96 \times \frac{3}{434} - 57.53 \times \frac{2}{434} = 1.021$$

Conclusions

In summary, we have found that, firstly, the new correlations show better agreement with experimental values compared with Keshavarz's latest empirical correlations as a whole, because amending factors have been introduced to probe the effect of the connective positions of groups to impact sensitivities. Secondly, the new correlations are simple and applicable to various nitro energetic compounds for quick estimation of impact sensitivities.

Acknowledgments

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