

One of the useful prediction methodologies for impact sensitivity is neural network architecture which can cover various types of energetic molecules. Cho et al. [16] used 17 molecular descriptors and showed subsets composed of compositional and topological descriptors provide better results than those composed of electronic descriptors including LUMO_MOPAC (Lowest Unoccupied Molecular Orbital from MOPAC), HOMO_MOPAC (Highest Occupied Molecular Orbital from MOPAC), Dipole_MOPAC (Dipole moment from MOPAC) and HF_MOPAC (Heat of Formation from MOPAC). The method of Cho et al. [16] cannot be used for insensitive explosives. It was recently found that some structural parameters can also be used to find out impact sensitivity by choosing only 10 molecular descriptors [2]. This method can be used for various types of $C_dH_bN_cO_d$ explosives including insensitive explosives.

Some simple relationships relate impact sensitivities with measured and predicted molecular properties which include the oxygen balance of the molecules [17–19], molecular electronegativities [20,21], vibrational states [22,23], molecular masses and detonation gas concentrations [24], parameters related to oxidation numbers [25], partial atomic charges [26,27], and structural factors [1–4].

Since there are large differences of impact sensitivities for different isomers of polynitroheteroarenes, it seems that predicting suitable correlation is difficult. However, large uncertainties associated with some of experimental data also hamper for explosives scientists to find good correlations for impact sensitivity of polynitroheteroarenes. High nitrogen content molecules such as nitroimidazoles, nitropyrazoles, nitrotriazoles and nitropyrimidines as potential energetic materials have different behaviors on impact. It was recently found that impact sensitivity of nitroheterocycles can most suitably be expressed as its elemental composition and the number of –CNC– and –CNNC– moieties in aromatic ring divided by molecular weight of explosive [4]. This correlation gives more reliable results compared to neural network method of Cho et al. [16] but it cannot be applied for insensitive explosives.

3. Results and discussion

Prediction of impact sensitivity is in large part a chemical problem. It is believed that hot spots in the energetic materials contribute to initiation in the drop weight impact test. Several factors contribute to the materials response to the stimulus in impact sensitivity tests. They include (1) the ease with which a detectable reaction of any kind can be initiated in an explosive; (2) the tendency of a small reaction, once established, to grow to destructive proportions; (3) the ease with which a high-order detonation can be established in an explosive. The formation and growth of hot spots could strongly affect the measurement which make the results sensitive to the conditions under which the tests are performed.

The studies on impact sensitivities of various polynitroheteroarenes including insensitive explosives have shown that it is possible to gain a general reliable correlation. It was found that combination of the number of carbons and hydrogens as well as contribution of the sum of specific structural parameters, which can increase or decrease the sensitivity of an explosive, are important factors. Thus, a general equation for prediction of impact sensitivity of polynitroheteroarenes with general formula $C_dH_bN_cO_d$ can be written as follows:

$$\log h_{50} = \frac{y_1 a + y_2 b + y_3 \sum SSP_i}{MW} \quad (1)$$

where SSP_i is the specific structural parameters that can decrease or increase impact sensitivity, y_1 – y_3 are adjustable parameters which can be found from experimental data given in Table 1 for various polynitroheteroarenes. Different polynitroheteroarenes given in Table 1 have various structural parameters. This situation is useful in getting more reliable correlation compared to previous

relationship [4] and neural network calculation [2]. It should be mentioned that a database archived by Storm et al. [28] was used in Table 1 because their collected data contain different molecular structures of polynitroheteroarenes. Moreover, since the measured data of impact sensitivity varied widely depending on instrumental types and to conditions of the experiments, the database of Storm et al. [28] was not augmented by others. In contrast to previous work [4] and artificial neural network scheme given by Cho et al. [16], data of insensitive explosives, whose experimental values are given as “greater than 320 cm”, have also been inserted in data. This condition removes restriction of predicting insensitive polynitroheteroarenes in mentioned methods. To predict adjustable parameters, the left-division method for solving linear equations uses the least squares method [29] because the equation set is overdetermined. The optimized relationship has the following form:

$$\log h_{50} = \frac{52.13a + 31.80b + 117.6 \sum SSP_i}{MW} \quad (2)$$

To get impact sensitivity for new polynitroarenes through Eq. (2), it would be needed to specify the value of SSP_i in the wished energetic molecule. The SSP_i can be specified according to molecular structures as

- (a) *The existence of amino derivatives as substituents in central heteroarene:* Amino derivatives (Ar–NH– or R–NH–) have main effect in decreasing of impact sensitivity of some explosives [10]. The effects of these substituents depend on molecular structure of central heteroarene so that the contributions of amino derivatives may be ignored for some cases. As representative examples, for central heteroarenes that contain four nitrogens (e.g. 1,2,3,4-terazole derivatives) and three nitrogens attached subsequently in one ring (e.g. 1,2,3-triazole derivatives) or nitropyrimidine explosives with attaching an aromatic ring to nitrogen (e.g. 1-picryl-2-picrylamino-1,2-dihydropyrimidine), the presence of amino derivatives have no notable effect and the value of SSP_i can be taken as zero. The values of SSP_i are 0.5, 0.6 and 2.5 for the presence of amino derivatives in nitropyridine, nitrofurazane (or nitrooxidazole) and nitro-1,2,4-triazole (or nitropyrimidine) explosives, respectively. For the other nitroheteroarenes that contain only nitrogen as hetero atoms, SSP_i can be taken as 2.0 in the presence of amino derivatives.

Impact sensitivities of explosives depend on the rates of thermal decomposition reactions which occur at temperature generated under the impact hammer. The rate-determining step for this process is usually being the homolytic cleavage of the weakest atom linkage that can be referred to as the “trigger linkage” by Kamlet and Adolph [19]. Some authors have tried to get correlations with experimental drop weight impact data for a wide range of explosives through quantum mechanical methods, e.g. Rice and Hare [30] or Haskins et al. [31]. However, introducing amino groups into a polynitroarenes is one of the simplest approach to improve the thermal stability and impact insensitivity of an explosive [10,30]. For example, 1,3,5-triamino-2,4,6-trinitrobenzene places at the top of the list of thermally stable and safe explosives. As seen for polynitroheteroarenes, the number of nitrogens and their arrangements in central heteroarene can cancel stabilizing effect of amino groups under certain conditions.

- (b) *Attaching an aromatic ring (e.g. picryl) to nitrogen and presence of one nitro group in specific position:* For nitroimidazole, nitropyrazole and nitro-1,2,4-triazole explosives, attaching an aromatic ring to nitrogen or the presence of nitro group in certain position can decrease impact sensitivity of mentioned compounds under certain conditions. However, the values of SSP_i are equal to 1.0 and 0.6 for attachment of aromatic ring

Table 1
Comparison of predicted h_{50} (cm) of new method and artificial neural network [2] with experimental data for various polynitroheteroarenes.

Compound	h_{50} (exp.) [29]	h_{50} (new method)	Dev	h_{50} (neural network)	Dev
2,4,6-Trinitropyridine-1-oxide	20	26	6	80	60
3,3',5,5'-Tetranitro-2,2'-azopyridine	56	60	4	95	39
2,6-Bis(picrylazo)-3,5-dinitropyridine	33	41	8	87	54
2,6-Bis(picrylamino)-3,5-dinitropyridine	63	76	13	107	44
3,5-Bis(picrylamino)-2,6-dinitropyridine	92	76	-16	107	15
2,6-Bis(picrylamino) pyridine	192	208	16	223	31
2,4,6-Trinitroimidazole	68	8	-60	44	-24
2,4-Dinitroimidazole	105	97	-8	84	-21
Ammonium-2,4,5-trinitroimidazole	50	19	-31	54	4
Ammonium-4,5-dinitroimidazole	77	63	-14	130	53
4,4',5,5'-Tetranitro biimidazole	37	16	-21	63	26
Diammonium-4,4',5,5'-tetranitro biimidazole	105	43	-62	98	-7
2,4-Dinitro-1-picrylimidazole	46	34	-12	154	108
2-Nitro-1-picrylimidazole	312	312	0	195	-117
4-Nitro-1-picrylimidazole	161	160	-1	195	34
1-Picrylimidazole	314	>320	6	286	-28
Ammonium-3,5-dinitropyrazole	158	161	3	130	-28
4-Nitro-1-picrylpyrazole	112	114	2	195	83
4-Nitro-3-picrylaminopyrazole	>320	>320	0	235	-85
3,5-Dinitro-1-methyl-4-picrylpyrazole	118	91	-27	144	26
3,5-Dinitro-1-methyl-4-picrylaminopyrazole	274	240	-34	217	-57
1,4-Dipicrylpyrazole	314	292	-22	188	-126
4-Nitro-1-picryl-3-picrylaminopyrazole	149	157	8	183	34
5-Nitro-1-picryl-4-picrylaminopyrazole	>320	284	-36	183	-137
3-Amino-4-nitrofurazan	27	20	-7	37	10
4,4'-Dinitro-3,3'-bifurazan	13	8	-5	12	-1
3-Nitro-4-picrylaminofurazan	60	51	-9	54	-6
3-Amino-4-picrylaminofurazan	120	120	0	128	8
2,5-Dipicryl-1,3,4-oxadiazole	20	55	35	27	7
3,4-Bis-(picrylamino) furazan	71	79	8	81	10
3,5-Bis-(picrylamino) 1,2,4-oxadiazole	95	79	-16	81	-14
3-Nitro-1,2,4-triazole	>320	319	-1	301	-19
3-Nitro-1,2,4-triazole-5-one	291	157	-134	236	-55
Ammonium 3-nitro-1,2,4-triazolate	>320	>320	0	>320	0
Ammonium 3,5-dinitro-1,2,4-triazolate	110	96	-14	112	2
4-Methyl-3,5-dinitro-1,2,4-triazole	155	137	-18	179	24
5,5'-Dinitro-3,3'-bi-1,2,4-triazole	153	176	23	222	69
4-(2-Nitroethyl)-3,5-dinitro-1,2,4-triazole	35	28	-7	66	31
3-Nitro-1-picryl-1,2,4-triazole	68	87	19	302	234
3-Picrylamino-1,2,4-triazole	>320	>320	0	255	-65
4-Picrylamino-1,2,4-triazole	314	320	6	302	-12
3-Amino-5-picrylamino-1,2,4-triazole	230	320	90	266	36
4-(2,4-Dinitrobenzyl)-3,5-dinitro-1,2,4-triazole	96	125	29	229	133
4-(4-Nitrobenzyl)-3,5-dinitro-1,2,4-triazole	>320	>320	0	>320	0
2-Picryl-3-picrylamino-1,2,4-triazole	320	252	-68	234	-86
3,5-Bispicrylamino-1,2,4-triazole	240	247	7	222	-18
N,N'-Dipicryl-5,5'-dinitro-3,3'-bi-1,2,4-triazole	138	70	-68	183	45
5,5'-Bispicrylamino-3,3'-bi-1,2,4-triazole	>320	225	-95	289	-31
4-Nitro-1,2,3-triazole	25	30	5	178	153
Ammonium 4-nitro-1,2,3-triazole	235	102	-133	235	0
4-Nitro-1-picryl-1,2,3-triazole	9	16	7	46	37
1-(3',5'-Dinitrophenyl)-4-nitro-1,2,3-triazole	56	33	-23	57	1
1-(3',4'-Dinitrophenyl)-4-nitro-1,2,3-triazole	51	33	-18	57	6
1-Picryl-1,2,3-triazole	10	33	23	57	47
2-Picryl-1,2,3-triazole	200	231	31	57	-143
1-(3'-Amino-2',4',6'-trinitrophenyl)-1,2,3-triazole	31	36	5	71	40
4-Picrylamino-1,2,3-triazole	103	90	-13	71	-32
4,6-Dinitro-1-picryl benzotriazole	40	33	-7	64	24
5,6-Dinitro-1-picryl benzotriazole	35	33	-2	64	29
1-Picryl-4-picrylamino-1,2,3-triazole	35	39	4	61	26
2,6-Dipicrylbenzo-[1,2-d:4,5-d']-bistriazole-4,8-dione	95	55	-40	48	-47
1,7-Dipicrylbenzo-[1,2-d:4,5-d']-bistriazole	38	55	17	55	17
1,5-Dipicrylbenzo-[1,2-d:4,5-d']-bistriazole	40	55	15	55	15
2,4,6,2',2'',4'',6''-Heptanitro-4',6''-diaza-m-terphenyl	58	65	7	167	109
2,4,6,4',2'',4'',6''-Heptanitro-2',6''-diaza-m-terphenyl	58	65	7	167	109
1-Picryl-2-picrylamino-1,2-dihydropyrimidine	106	111	5	214	108
5-Nitro-2,4,6-tris-(picrylamino)-pyrimidine	201	142	-59	184	-17
rms deviation (cm)			36		66

to nitrogen in imidazole (or only in mononitro imidazol) and nitropyrazole explosives, respectively, except for the existence of only two aromatic substituents attached to heteroarene ring without further substituents so that $SSP_i = 2$ in this situation. The existence of polynitrophenyl as an attachment on

nitrogen atom at 4-position for 1,2,4-triazole explosives (e.g. 4-(2,4-dinitrobenzyl)-3,5-1,2,4-triazole) can decrease impact sensitivity so that the value of SSP_i is equal to 0.7 for this state. The values of SSP_i are 0.6, 0.8 and 1.0 for the existence of one nitro group in positions of 2 in 3 (or 5) in nitropyrazole, nitroim-

Table 2
Comparison of predicted h_{50} (cm) of new method with experimental data for miscellaneous and new polynitroheteroarenes.

Compound	h_{50} (exp.)	h_{50} (new method)	Dev
Ammonium 5-nitro-tetrazolate	30 [28]	23	-7
Ethylenediammonium di-5-nitrotetrazolate	42 [28]	65	23
3,5-Dinitroisoxazole	29 [28]	15	-14
1,4-Dinitroglycoluril	100 [28]	28	-72
1-Nitro-2,5-bis-(trinitromethyl)-pyrrolidine	6 [28]	16	10
5-Picrylaminetetrazole	36 [28]	46	10
3,3,9,9-Tetranitro-1,5,7,11-tetraoxaspiro-(5,5)-undecane	66 [28]	66	0
N-(2,2,2-Trinitroethyl)-3,3,5,5-tetranitro-piperidine	18 [28]	28	10
N-(Trinitropropyl)-3,3,5,5-tetranitro-piperidine	29 [28]	46	17
1,3,7,9-Tetranitrodibenzo-1,3a,4,6a-tetraazapentalene	85 [28]	87	2
3,6-Bis-(picrylamino)-s-tetrazine	61 [28]	53	-8
1,3,5-Tris(1-oxo-5,5,5-trinitro-3-nitrazapentyl)-s-triazacyclohexane	13 [28]	34	21
Tripicryl-s-triazene	85 [28]	63	-22
2,4,6-Tris(3,5-diamino-2,2,4,6-triphenylamino)-1,3,5-triazine	170 [8]	134	-36
4,4'-Dinitro-3,3'-diazenufuroxane	>320 [8]	>320	0
4,4'-Dinitro-3,3'-bifurazan	12 [10]	8	-4
rms deviation (cm)			24

imidazole and 3 in nitro-1,2,4-triazole explosives, respectively. It should be mentioned that this condition is valid for nitroimidazole up to only disubstituted nitroimidazole explosives. As representative example for this part, $\sum SSP_i$ is equal to 1.8 for 2-nitro-1-picryl-imidazole meanwhile the value $\sum SSP_i$ becomes 1.0 for 4-nitro-1-picryl-imidazole as the other isomer.

If “trigger linkage” could be identified, and avoided, less sensitive materials could be designed [32]. The belief of explosive chemists is that ammonium salts are “unusually stable” because when an acid is converted to its ammonium salt three extra hydrogens are added the ammonium salt will be less sensitive than the present acid [28]. Since 1,2,4-triazoles are a class less sensitive, it appears that ammonium counter ion provides no special insensitivity. This condition has also been confirmed by Storm et al. [28]. In less sensitive derivatives of nitroimidazole, nitropyrazole and nitro-1,2,4-triazole explosives complex chemistry is likely to proceed a rate determining step and the insensitivity of the explosive is in fact the consequence of the chemistry proceeding the rate determining step. Because of considerable delocalization of charge through $-N=N-$ and $-C=C-$ double bonds caused by different resonating structure, the insensitivity to impact and a high-level of thermal stability may be accounted for some isomers of polynitroheteroarenes including nitroimidazole, nitropyrazole and nitro-1,2,4-triazole explosives.

- (c) *Increasing of impact sensitivity of nitro-1,2,3-triazole explosives:* The attachment of an aromatic ring to nitrogen in position 1 can increase impact sensitivity so that the value of SSP_i is equal to -1.0 in this case. As mentioned in part (a), this condition is valid for the absence of amino derivatives.

If one of substituents in polynitroheteroarenes contains another more active site for initiation of decomposition, e.g. $R-NO_2$, the value of $\sum SSP_i$ can be taken as zero.

The sensitivity to impact and instability varies from isomer to isomer in nitro-1,2,3-explosives because of the presence of shorter and stronger N–N bonds which facilitate decomposition through the loss of N_2 [33]. For example, there are large differences in impact sensitivities of 1-picryl-1,2,3-triazole compared to 2-picryl-1,2,3-triazole and 4-nitro-1-picryl-1,2,3-triazole compared to 4-nitro-1-picryl-1,2,3-triazole which can be ascribed to facile loss of nitrogen in the 1-picryl isomers [33]. This state provides clues to decomposition mechanisms through lose nitrogen of more sensitive isomers by a low activation energy, exothermic, process. Besides, it gains propagating the hot spot in which the N_2 loss is certainly a “trigger linkage”.

Recent artificial neural network [2], which give more reliable predictions compared to complex quantum mechanical method [30], were used to confirm the reliability of predicted results. As shown in Table 1, the predicted results show a good agreement with experimental values (rms = 36 cm) compared to the outputs of neural network (rms = 66 cm). Therefore, Eq. (2) provides good predictions with respect to the results of complex neural network architecture. To check the reliability of this method for further explosives, some miscellaneous nitroheterocyclic explosives and several new synthesized polynitroheteroarenes are also given in Table 2. As seen, the predicted results have give good results compared to experimental data (rms = 24 cm). Thus, comparison of calculated results with experimental data listed in Tables 1 and 2 may be taken as suitable confirmation of the new simple correlation for different polynitroheteroarenes including nitropyridine, nitroimidazole, nitropyrazole, nitrofurazane, nitrooxadiazole, nitro-1,2,4-triazole, nitro-1,2,3-triazole and nitropyrimidine explosives.

4. Conclusions

A new method for prediction of impact sensitivity of polynitroheteroarenes has been introduced. The main intent in this work was to research the likelihood of a generalized method to evaluate impact sensitivity of polynitroheteroarenes that have received a great amount of interest. The present method uses only the number of carbons and hydrogens as well as specific structural parameters that can be easily got from molecular structure. The proposed method is superior to that of neural network and quantum mechanical method in terms of accuracy, generality and simplicity. It is more reliable than previous work [4] and can be applied for insensitive polynitroheteroarenes. As can be seen in Tables 1 and 2, the predicted results by the new method are comparable with the outputs of complicated neural network architecture and the accuracy of prediction is not necessarily improved by greater complexity.

Acknowledgement

We would like to thank the research committee of Malek-ashtar University of Technology (MUT) for supporting this work.

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