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Investigation of the Various Structure Parameters for Predicting Impact Sensitivity of Energetic Molecules via Artificial Neural Network

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Abstract

A generalized scheme is introduced for predicting impact sensitivity of any explosives by using artificial neural networks. Experimental values for the impact sensitivity for 291 compounds containing C, H, N and O have been used for training and testing sets. The input descriptors include aromatic character, heteroaromatic character, the number of $N-NO_2$ bonds and the number of α-hydrogen atoms as well as the number of carbon, hydrogen, nitrogen, and oxygen divided by molecular weight. The reliability of the proposed model was assessed by comparing the results against measured values as well as five models of complicated quantum mechanical computed values of 14 CHNO explosives from a variety of chemical structures. The model gives root mean squares errors of 41 cm and 56 cm for training and test sets, respectively, of the H_{50} quantity.

Keywords: Impact Sensitivities, Neural Network, $C_aH_bN_cO_d$ Explosives, Detonation, Safety

1 Introduction

The development, manufacture, testing and fielding of new energetic materials are lengthy and expensive due to the heavy reliance on experimentation and measurement of a variety of candidate materials, from which only a few will be selected as most suitable to meet specified objectives. It is hoped that the development capabilities to predict various properties, which are associated with performance and sensitivity of a notional energetic material, would be improved before expanding resources in its synthesis. Elimination of any poor candidate of energetic materials due to sensitivity or performance through predictive capabilities at early stages of development is highly desirable. Recently, some approaches have been introduced for predicting detonation parameters of different classes of explosives, which can determine reliable performance of energetic materials by some simple procedures [1 – 12].

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Some stimuli, which includes impact, shock, heat, electrostatic discharge and friction, can cause detonation. The impact sensitivity is usually measured by drop-weight impact test, where a 2.5 kg mass is dropped from a predetermined height onto the striker plate and evidence of reaction or no reaction is recorded. A sequence of tests is carried out until the impact sensitivity or the sensitivity index, H_{50}, is obtained. The H_{50} value is the height that a given mass must be dropped onto the sample to produce an explosion of 50% of the test trial. The results are often not reproducible, and in some cases reported data gives widely varying H_{50} values, e.g. H_{50} values for two recrystallized 2,4,6-Trinitrotoluene vary from below 100 cm to above 250 cm [13]. It is believed that hot spots in the energetic material contribute to initiation in the drop weight impact test. Since the formation and growth of hot spots could strongly affect the measurements, the results are extremely sensitive to conditions under which the tests are performed.

The neural network has been applied widely to various areas of science and engineering. Some examples include the modeling of such petroleum processes as the hydro cracker [14], the prediction of thermodynamic and the transport properties of pure components [15] and the structural group contribution method for predicting pure component auto ignition temperature [16]. The neural network of computation has several advantages for solving complicated problems especially in the speed of computation, learning ability and fault tolerance. Theoretical background of neural computing has been given elsewhere [17, 18].

This work demonstrates that the complex impact sensitivity can be modeled by back propagation neural network. Considering the difficulty and large uncertainty of different measurements by users, neural network can be an effective alternative. The composition and various structural factors approach presented here is novel and proves to be a powerful tool for predicting the impact sensitivity of pure explosives from only their molecular structure. We are

currently developing a method for estimating the impact sensitivities of explosives, utilizing the current procedure for automatic generation and reliable estimation of new proposed explosive for which no data exist. In spite of the fact that many methods for predicting impact sensitivities have been developed, a generalized method is still needed for the explosive users in industry. The aim of this work was to study other alternatives for evaluation of impact sensitivities of explosives. Since there is no need to know or establish a mathematical model, artificial neural network represent so-called "soft" modeling. The purpose of this work was to study the possibility of applying artificial neural network for impact sensitivity computation from a general point of view for any kind of data. If we have trained a neural network, it is possible to predict the required parameters immediately.

2 Prediction Methods Other than Neural Network

Despite all uncertainties associated with the impact sensitivity tests, there exist numerous measurements for pure explosives and they are considered to provide only a crude and qualitative estimate of an explosive's sensitivity. Thus, the impact sensitivity results are considered to be suspect. But most of the studies that attempt to associate molecular properties with sensitivities rely on drop weight impact measurements [13, 19–51].

Some simple relationships relate impact sensitivities with measured and predicted molecular properties which include the oxygen balance of the molecules [13, 19], molecular electronegativities [26, 27], vibrational states [29, 30], molecular masses and detonation gas concentrations [24], parameters related to oxidation numbers [28], partial atomic charges [21–23, 26, 38, 39], heats of reaction [31, 32], heats of explosion [25], activation energies [25, 31–36, 43] and bond orders [33–35]. Politzer and coworkers [40, 46–50] have identified a few features of electrostatic potentials using quantum mechanical calculations for $C_aH_bN_cO_d$ explosives that appear to be related to their sensitivity to impact. Rice and Hare [51] used approximations to the electrostatic potential at midpoints, statistical parameters of these surface potentials and the property-structure relation method "generalized interaction property function" (GIPF) or computed heats of detonation to predict impact sensitivity of $C_aH_bN_cO_d$ explosives. Five introduced models use parameters related to features of the surface electrostatic potentials, which can be summarized as below:

Model I: The approximate electrostatic potential at the midpoint of each bond, $\bar{V}_{mid}$, 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_2 which is

$$\bar{V}_{mid} = \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{n}\frac{q_j}{r_{ij}} \tag{1}$$

where n is the number of atoms in the molecule, N is the number of bonds in the molecule for which electrostatic potentials of midpoints of the bonds were calculated, q_j is 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 suitable function for calculation of H_{50} in this case is:

$$H_{50}(/cm) = 63.6 + 1.89\cdot 10^4\cdot\exp(-0.0210\,mol/kJ \cdot \bar{V}_{mid}) - 0.08783\,mol/kJ\cdot\bar{V}_{mid} \tag{2}$$

Model II: This model is based on the difference between the magnitudes of the averages of the positive and negative values of the electrostatic potential on the isosurface, $\left|\bar{V}^+ - \left|\bar{V}^-\right|\right|$, and one obtains:

$$H_{50}(/cm) = 9.2 + 8.03\cdot 10^2 \cdot\exp\left[-\left(0.0875\,mol/kJ\cdot\left|\bar{V}^+ - \left|\bar{V}^-\right|\right|\right)\right] \tag{3}$$

Model III: This model depends on another statistical quantity associated with the electrostatic potential of the molecule, the balance parameter ν. The following equation was obtained from best fit of data:

$$H_{50}(/cm) = 29.3 + 1.386\cdot 10^{-3}\cdot\exp[48.84\cdot\nu] \tag{4}$$

Model IV: The use of computed heats of detonation, Q_d, in kJ/g can lead the following equation by GIPF:

$$H_{50}(/cm) = 27.8 + 0.1135\cdot\exp[-(2.6479\,g/kJ[Q_d - 6.9496\,kJ/g])] \tag{5}$$

Model V: This model combines the exponential dependencies of both the GIPF balance parameter ν and Q_d in the following equation:

$$H_{50}(/cm) = 1.341\cdot\exp(8.1389\nu - 1.6234\,g/kJ[Q_d - 6.166\,kJ/g]) \tag{6}$$

3 Application of Artificial Neural Network for Determining Impact Sensitivities

The structural dependency of impact sensitivity using an artificial neural network model was investigated. The model was instructed and tested with MATLAB code [52] with a large number of $C_aH_bN_cO_d$ explosives. Several artificial neural network architectures were tried and the one that best simulated the impact sensitivity was retained. The final neural structure is shown in Figure 1 that consists of the three layers input, output, and hidden. The input layer has a number of descriptors, which was equal to ten here. The network is composed of fully connected two layers: 10 input nodes, fifteen hidden-layer neurons and a single output neuron corresponding to impact sensitivity of explosive. Considering a broader range of structural variety of

explosive compounds in this study, some of the important factors that can affect the sensitivity of explosive are chosen as descriptors. The following ten structural descriptors were used for neural network modeling for any $C_aH_bN_cO_d$ explosive: (1) a/MW; (2) b/MW; (3) c/MW; (4) d/MW; indicator variables for (5) aromaticity; (6, 7) heteroaromaticity (N and O); (8) N–NO_2; (9) α-hydrogen; (10) salt. For indicator variables, values of 1 or 0 are assigned for the presence or absence of the cases (5), (7), (8) and (10) except for cases (6) and (9) where indicator variables were set to 2 for their presence. The value ranges of above indicators are presented in Table 1. A sigmoid function was used as the transfer function for each neuron. If a certain input in the network did not exist in a molecule an input value of zero was assigned to that input. The connection weights of the network were adjusted iteratively by back propagation algorithm. The average absolute deviation, maximum deviation and the correlation coefficient of the predictions along with the corresponding iterative steps (epochs) were recorded during the learning course. It is found that 300 epochs were sufficient to achieve the convergence of learning. In this case the deviation between the actual and desired responses has no significant change, thus the training was terminated at that number of iteration steps. We learned that the best number of hidden layer units is 15. The operation of the output layer is linear which can be given as:

$$y_k(x) = \sum_j w_{kj} h_j(x) + b_k \tag{7}$$

where y_k is the k-th output unit for input vector x, w_{kj} is the weight connection between k-th output unit and the j-th hidden layer unit $h_j(x)$ and b_k is the bias. The overall performance of neural network is evaluated in terms of root mean squared error (RMS) and relative RMS according to the equations below:

$$RMS = \sqrt{\frac{\sum_k^n (y_k - y_k')^2}{n}} \tag{8}$$

$$RMS - relative = 100\% \cdot \sqrt{\frac{\sum_k^n \left(\frac{y_k - y_k'}{y_k}\right)^2}{n}} \tag{9}$$

where y_k is the desired output (means measured data of test set) and y'_k is the actual output of the network and n is the number of explosive compounds in analyzed set.

The predictive ability of the artificial neural network can be demonstrated by training it with only 275 of experimental data after arriving at the best network architecture. The trained network was then applied to predict impact sensitivity of 14 remaining explosives in the test set, which were not included in the learning data base. The predicted results of impact sensitivities of training and test sets are given in Tables 2 and 3, respectively. The results indicate that the model obtained can correctly represent structural-impact sensitivities relationships of various $C_aH_bN_cO_d$ explosives. The used molecular descriptors obtained solely from the structures can represent the structural features of explosives responsible for their impact sensitivities. The results of the test set are also compared with five models using complicated quantum mechanical computation. As can be seen in Table 3, the predictions of the neural network model for the test data set are better compared to quantum mechanical models.

Thus, as indicated in Figure 1, the neural network parameters contain 10 input neurons for ten descriptors as well as 15 hidden-layer neurons plus a bias and one output neuron namely impact sensitivity.

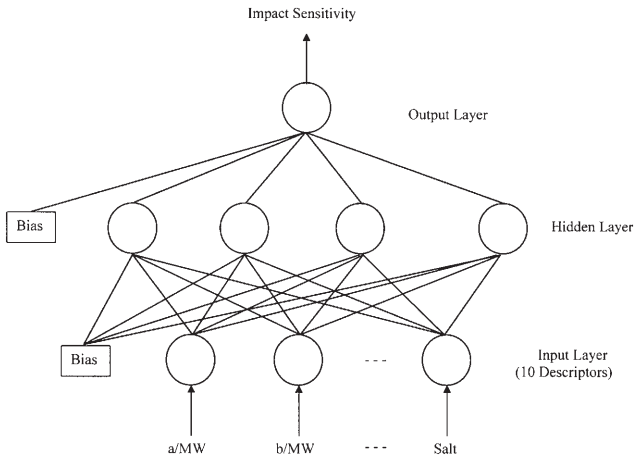

Figure 1. Architecture of artificial neural network for predicting impact sensitivity of explosive from its structure.

Table 1. Ranges of molecular descriptors covered by different classes of explosives in the training set of 277 compounds.

Variables	Absence/Presence
Aromaticity	0/1
N–NO_2	0/1
Heteroaromaticity (N)	0/2 × Number of N atoms in heteroaromatic ring
Heteroaromaticity (O)	0/ Number of O atoms in heteroaromatic ring
α-Hydrogen	0/2
Salt	0/1

4 Conclusions

Recently there is growing interest in the application of the artificial neural network in quantitative structure-property relationships that quantify the structure and properties of molecules and allow the prediction of properties from structural parameters. A new method for prediction of impact sensitivity using artificial neural network has been presented. The training data for neural network of multilayer perceptions contains patterns of inputs together with the corresponding outputs, and the network learns to infer a

Table 2. Finally by the neural network obtained (predicted) and experimental H_{50} values (cm) of explosive compounds of training set.

No.	Compound	Formula	H_{50} (exp.)[a] (cm)	H_{50} (pred.)[b] (cm)
1	Hexanitrobenzene	$C_6N_6O_{12}$	11	6(5)
2	Pentanitrobenzene	$C_6HN_5O_{10}$	11	10(1)
3	1,2,3,5-Tetranitrobenzene	$C_6H_2N_4O_8$	28	24(4)
4	1,3,5-Trinitrobenzene	$C_6H_3N_3O_6$	71	108(−37)
5	2,4,6-Trinitrophenol	$C_6H_3N_3O_7$	64	97(−33)
6	Pentanitroaniline	$C_6H_2N_6O_{10}$	22	14(8)
7	2,3,4,6-Tetranitroaniline	$C_6H_3N_5O_8$	47	50(−3)
8	2,4,6-Trinitroaniline	$C_6H_4N_4O_6$	141	172(−31)
9	1,3-Diamino-2,4,6-trinitrobenzene	$C_6H_5N_5O_6$	320	290(30)
10	1,3,5-Triamino-2,4,6-trinitrobenzene	$C_6H_6N_6O_6$	490	337(153)
11	Hexanitrobiphenyl	$C_{12}H_4N_6O_{12}$	70	55(15)
12	3,3′-Diamino-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{12}H_6N_8O_{12}$	67	102(−35)
13	4,4′-Diamino-2,2′,3,3′,5,5′,6,6′-octanitrobiphenyl	$C_{12}H_4N_{10}O_{16}$	57	20(37)
14	4,6-Dinitrobenzofuroxan	$C_6H_3N_4O_6$	76	53(23)
15	7-Amino-4,6-dinitrobenzofuroxan	$C_6H_3N_5O_6$	100	134(−34)
16	5,7-Diamino-4,6-dinitrobenzofuroxan	$C_6H_4N_6O_6$	120	177(−57)
17	7-Amino-4,5,6-trinitrobenzofuroxan	$C_6H_2N_6O_8$	56	38(18)
18	Benzotrifuroxan	$C_6N_6O_6$	53	31(22)
19	Pentanitrotoluene	$C_7H_3N_5O_{10}$	18	25(−7)
20	2,3,4,5-Tetranitrotoluene	$C_7H_4N_4O_8$	15	43(−28)
21	2,3,4,6-Tetranitrotoluene	$C_7H_4N_4O_8$	19	43(−24)
22	2,3,5,6-Tetranitrotoluene	$C_7H_4N_4O_8$	25	43(−18)
23	2,4,6-Trinitrotoluene	$C_7H_5N_3O_6$	98	112(−14)
24	2,3,4-Trinitrotoluene	$C_7H_5N_3O_6$	56	112(−56)
25	3,4,5-Trinitrotoluene	$C_7H_5N_3O_6$	107	112(−5)
26	2-Amino-3,4,5,6-tetranitrotoluene	$C_7H_5N_5O_8$	36	44(−8)
27	3-Amino-2,4,5,6-tetranitrotoluene	$C_7H_5N_5O_8$	37	44(−7)
28	4-Amino-2,3,5,6-tetranitrotoluene	$C_7H_5N_5O_8$	47	44(3)
29	2,2′,4,4′,6,6′-Hexanitrodiphenylmethane	$C_{13}H_6N_6O_{12}$	39	53(−14)
30	2-Azido-1,3,5-trinitrobenzene	$C_6H_2N_6O_6$	19	61(−42)
31	Azidopentanitrobenzene	$C_6N_8O_{10}$	17	52(−35)
32	2-Diazo-4,6-dinitrophenol	$C_6H_2N_4O_5$	9	52(−43)
33	3-Methyl-2-diazo-4,5,6-trinitrophenol	$C_7H_3N_5O_7$	8	10(−2)
34	N-Methyl-N,2,4,6-tetranitroaniline	$C_7H_5N_5O_8$	25	31(−6)
35	N-Methyl-2-amino-N,3,4,5,6-pentanitrotoluene	$C_8H_6N_6O_{10}$	21	28(−7)
36	N-Methyl-3-amino-N,2,4,5,6-pentanitrotoluene	$C_8H_6N_6O_{10}$	18	28(−10)
37	1,2,4,5-Tetranitrobenzene	$C_6H_2N_4O_8$	27	24(3)
38	2,3,4,5,6-Pentanitroaniline	$C_6H_2N_6O_{10}$	15	14(1)
39	1,3,5-Ttrinitrobenzene	$C_6H_3N_3O_6$	100	108(−8)
40	2,4,6-Ttrinitroresorcinol	$C_6H_3N_3O_8$	43	79(−36)
41	2,4,6-Ttrinitrophloro-glucinol	$C_6H_3N_3O_9$	27	61(−34)
42	2,3,4,6-Tetranitroaniline	$C_6H_3N_5O_8$	41	50(−9)
43	2,4-Dinitroresorcinol	$C_6H_4N_2O_6$	296	227(69)
44	4,6-Dinitroresorcinol	$C_6H_4N_2O_6$	320	227(93)
45	2,4,6-Trinitroaniline	$C_6H_4N_4O_6$	177	172(5)
46	2,4,6-Trinitro-3-aminophenol	$C_6H_4N_4O_7$	138	122(16)
47	1,3-Diamino-2,4,6-trinitrobenzene	$C_6H_5N_5O_6$	320	290(30)
48	1- Hydroxyl-3,5-Diamino-2,4,6-trinitrobenzene	$C_6H_5N_5O_7$	120	186(−66)
49	Ammonium picrate	$C_6H_6N_4O_7$	135	257(−122)
50	1,3,5-Triamino-2,4,6-trinitrobenzene	$C_6H_6N_6O_6$	320	337(−17)
51	2,4,6-trinitrobenzonitrile	$C_7H_2N_4O_6$	140	60(80)
52	2,4,6-trinitrobenzoic acid	$C_7H_3N_3O_8$	109	102(7)
53	2,4,6-trinitroanisole	$C_7H_5N_3O_7$	192	216(−24)
54	3-Methoxy-2,4,6-Trinitroaniline	$C_7H_6N_4O_7$	320	259(61)
55	1,3-Dimethoxy-2,4,6-trinitrobenzene	$C_8H_7N_3O_8$	251	284(−33)
56	2′,2′,2′-trinitroethyl-2,4,6-trinitrobenzoate	$C_9H_4N_6O_{14}$	24	27(−3)
57	2′,2′,2′-trinitroethyl-3,5-dinitrobenzoate	$C_9H_5N_5O_{12}$	73	83(−10)
58	2′,2′,2′-trinitroethyl-3,5-dinitrosalicylate	$C_9H_5N_5O_{13}$	45	71(−26)
59	1,4,5,8-tetranitro-napthalene	$C_{10}H_4N_4O_8$	100	101(−1)
60	2′,2′-dinitropropyl-2,4,6- trinitrobenzoate	$C_{10}H_7N_5O_{12}$	214	156(58)
61	2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{12}H_4N_6O_{12}$	85	55(30)
62	3-hydroxy-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{12}H_4N_6O_{13}$	42	59(−17)
63	3,3′-dihydroxy-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{12}H_4N_6O_{14}$	40	56(−16)
64	2,2′,4,4′,6,6′-hexanitro-diphenylamine	$C_{12}H_5N_7O_{12}$	48	62(−14)
65	3,3′-diamino-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{12}H_6N_8O_{12}$	132	102(30)
66	2,2′,4,4′,6-pentanitro-benzophenone	$C_{13}H_4N_5O_{11}$	54	79(−25)

Table 2. (cont.)

No.	Compound	Formula	H_{50} (exp.)[a] (cm)	H_{50} (pred.)[b] (cm)
67	2,2′,2″,4,4′,4″,6,6′,6″-nonanitro-m-terphenyl	$C_{18}H_5N_9O_{18}$	39	41(−2)
68	2,2″,4,4′,4″,6,6′,6″-Octanitro-m-terphenyl	$C_{18}H_6N_8O_{16}$	63	66(−3)
69	2,2′,2″,4,4″,5′,6,6″-Octanitro-p-terphenyl	$C_{18}H_6N_8O_{16}$	40	66(−26)
70	2,2′,2″,4,4″,6,6′,6″-Octanitro-p-terphenyl	$C_{18}H_6N_8O_{16}$	59	66(−7)
71	Dodecanitroquaterphenyl	$C_{24}H_6N_{12}O_{24}$	40	36(4)
72	Azo-bis-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{24}H_6N_{14}O_{24}$	40	17(23)
73	2,4,6-trinitrobenzaldehyde	$C_7H_3N_7O_7$	36	49(−13)
74	2,4,6-trinitrobenzaldoxime	$C_7H_4N_4O_7$	42	40(2)
75	2,4,6-trinitrotoluene	$C_7H_5N_3O_6$	160	112(48)
76	1-Dinitromethyl-3-nitrobenzene	$C_7H_5N_3O_6$	105	112(−7)
77	2,4,6-trinitrobenzylalcohol	$C_7H_5N_3O_7$	52	93(−41)
78	2,4,6-trinitro-m-cresol	$C_7H_5N_3O_7$	191	93(98)
79	1-(2,2,2-trinitroethyl)-2,4,6-trinitrobenzene	$C_8H_4N_6O_{12}$	13	19(−6)
80	2,4,6-trinitrostyrene	$C_8H_5N_3O_6$	32	125(−93)
81	1-(2,2,2-trinitroethyl)-2,4-dinitrobenzene	$C_8H_5N_5O_{10}$	31	32(−1)
82	3,5-Dimethyl-2,4,6-trinitrophenol	$C_8H_7N_3O_7$	77	184(−107)
83	1-(3,3,3-trinitropropyl)-2,4,6-trinitrobenzene	$C_9H_6N_6O_{12}$	21	22(−1)
84	1-(3,3,3-trinitropropyl)-2,4-dinitrobenzene	$C_9H_7N_5O_{10}$	31	72(−41)
85	3-methyl-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{13}H_6N_6O_{12}$	53	53(0)
86	3-methyl-2,2′,4,4′,6-pentanitrobiphenyl	$C_{13}H_7N_5O_{10}$	143	93(50)
87	Hexanitrostilbene	$C_{14}H_6N_6O_{12}$	39	54(−15)
88	2,2′,4,4′,6,6′-hexanitrobibenzyl	$C_{14}H_8N_6O_{12}$	114	80(34)
89	3,3′-Dimethyl-2,2′,4,4′,6,6′-hexanitrobiphenyl	$C_{14}H_8N_6O_{14}$	135	71(64)
90	2,4,6-Trinitropyridine-1-oxide	$C_5H_2N_4O_7$	20	80(−60)
91	3,3′,5,5′-tetranitro-2,2′-azopyridine	$C_{10}H_4N_8O_8$	56	95(−39)
92	2,6-bis(picrylazo)-3,5-dinitropyridine	$C_{17}H_5N_{13}O_{16}$	33	87(−54)
93	2,6-bis(picrylamino)-3,5-dinitropyridine	$C_{17}H_7N_{11}O_{16}$	63	107(−44)
94	3,5-bis(picrylamino)-2,6-dinitropyridine	$C_{17}H_7N_{11}O_{16}$	92	107(−15)
95	2,6-bis(picrylamino) pyridine	$C_{17}H_9N_9O_{12}$	192	223(−31)
96	2,4,6-Trinitroimidazole	$C_3HN_5O_6$	68	44(24)
97	2,4-Dinitroimidazole	$C_3H_2N_4O_4$	105	84(21)
98	Ammonium-2,4,5-trinitroimidazole	$C_3H_4N_6O_6$	50	54(−4)
99	Ammonium-4,5-dinitroimidazole	$C_3H_5N_5O_4$	77	130(−53)
100	4,4′,5,5′-Tetranitro biimidazole	$C_6H_2N_8O_8$	37	63(26)
101	Diammonium-4,4′,5,5′-tetranitro biimidazole	$C_6H_8N_{10}O_8$	105	98(7)
102	2,4-Dinitro-1-picrylimidazole	$C_9H_3N_7O_{10}$	46	154(−108)
103	2-Nitro-1-picrylimidazole	$C_9H_4N_6O_8$	312	195(117)
104	4-Nitro-1-picrylimidazole	$C_9H_4N_6O_8$	161	195(−34)
105	1-Picrylimidazole	$C_9H_5N_5O_6$	314	286(28)
106	Ammonium-3,5-dinitropyrazole	$C_3H_5N_5O_4$	158	130(28)
107	4-Nitro-1-picrylpyrazole	$C_9H_4N_6O_8$	112	195(−83)
108	4-Nitro-3-picrylaminopyrazole	$C_9H_5N_7O_8$	320	235(85)
109	3,5-Dinitro-1-methyl-4-picrylpyrazole	$C_{10}H_5N_7O_{10}$	118	144(−26)
110	3,5-Dinitro-1-methyl-4-picrylaminopyrazole	$C_{10}H_6N_8O_{10}$	274	217(57)
111	1,4-Dipicrylpyrazole	$C_{15}H_6N_8O_{12}$	314	188(126)
112	4-Nitro-1-picryl-3-picrylaminopyrazole	$C_{15}H_6N_{10}O_{14}$	149	183(−34)
113	5-Nitro-1-picryl-4-picrylaminopyrazole	$C_{15}H_6N_{10}O_{14}$	320	183(137)
114	3-Amino-4-nitrofurazan	$C_2H_2N_4O_3$	27	37(−10)
115	4,4′-Dinitro-3,3′-bifurazan	$C_4N_6O_6$	13	12(1)
116	3-Ninitro-4-picrylaminofurazan	$C_8H_3N_7O_9$	60	54(6)
117	3-Amino-4-picrylaminofurazan	$C_8H_5N_7O_7$	120	128(−8)
118	2,5-Dipycryl-1,3,4-oxadiazole	$C_{14}H_4N_8O_{13}$	20	27(−7)
119	3,4-bis-(picrylamino) furazan	$C_{14}H_6N_{10}O_{13}$	71	81(−10)
120	3,5-bis-(picrylamino) 1,2,4-oxadiazole	$C_{14}H_6N_{10}O_{13}$	95	81(14)
121	2,4,6,2′,2″,4″,6″-heptanitro-4′,6′-diaza-m-terphenyl	$C_{16}H_5N_9O_{14}$	58	167(−109)
122	2,4,6,4′,2″,4″,6″-heptanitro-2′,6′-diaza-m-terphenyl	$C_{16}H_5N_9O_{14}$	58	167(−109)
123	1-picryl-2-picrylamino-1,2-dihydropyrimidine	$C_{16}H_7N_9O_{12}$	106	214(−108)
124	5-nitro-2,4,6-tris-(picrylamino)- pyrimidine	$C_{22}H_9N_{15}O_{20}$	201	184(17)
125	1,1,1,3-tetranitrobutane	$C_4H_6N_4O_8$	33	36(−3)
126	1,1,1,3,5,5,5-heptanitropentane	$C_5H_5N_7O_{14}$	8	16(−8)
127	1,1,1,6,6,6-hexanitro-3-hexyne	$C_6H_4N_6O_{12}$	7	19(−12)
128	1,1,1,6,6,6-hexanitro-3-hexene	$C_6H_6N_6O_{12}$	17	26(−9)
129	3,3,4,4-tetranitrohexane	$C_6H_{10}N_4O_8$	80	117(−37)
130	2,2,4,4,6,6-hexanitroheptane	$C_7H_{10}N_6O_{12}$	29	43(−14)
131	2,2,4,6,6-pentanitroheptane	$C_7H_{11}N_5O_{10}$	56	80(−24)
132	2,2,2-Trinitroethylcarbamate	$C_3H_4N_4O_8$	18	10(8)

Table 2. (cont.)

No.	Compound	Formula	H_{50} (exp.)[(a)] (cm)	H_{50} (pred.)[(b)] (cm)
133	2,2-Dinitro-1,3-propanediol	$C_3H_6N_2O_6$	110	107(3)
134	Methyl-2,2,2-trinitroethyl carbonate	$C_4H_5N_3O_9$	28	27(1)
135	4,4,4-Trinitrobutyramide	$C_4H_6N_4O_7$	40	41(−1)
136	Bis-(2,2,2-trinitroethyl)-carbonate	$C_5H_4N_6O_{15}$	16	10(6)
137	Methylene-bis-N,N′-(2,2,2-trinitroacetamide)	$C_5H_4N_8O_{14}$	9	9(0)
138	Bis-(trinitroethoxy)-methane	$C_5H_6N_6O_{14}$	17	14(3)
139	N,N′-Bis-(2,2,2-trinitroethyl)-urea	$C_5H_6N_8O_{13}$	17	12(5)
140	5,5,5-Trinitropentanone-2	$C_5H_7N_3O_7$	125	73(52)
141	Ethyl-2,2,2-trinitroethyl carbonatesize	$C_5H_7N_3O_9$	81	142(−61)
142	N-(2-propyl)-trinitroacetamide	$C_5H_8N_4O_7$	112	90(22)
143	Bis-(trinitroethyl)-oxalate	$C_6H_4N_6O_{16}$	15	14(1)
144	2,2,2-Trinitroethyl-4,4,4-trinitrobutrate	$C_6H_6N_6O_{14}$	18	18(0)
145	Bis-(trinitroethyl)-oxamide	$C_6H_6N_8O_{14}$	13	21(−8)
146	Trinitroethyl-2,2-dinitropropylcarbonate	$C_6H_7N_5O_{13}$	15	25(−10)
147	N-Trinitroethyl-4,4,4-trinitrobutramide	$C_6H_7N_7O_{13}$	18	11(7)
148	1,5-Bis-(trinitroethyl)-biuret	$C_6H_7N_9O_{14}$	24	10(14)
149	N-(t-Butyl)-trinitroacetamide	$C_6H_{10}N_4O_7$	110	168(−58)
150	Tris-(2,2,2-trinitroethyl)-orthoformate	$C_7H_7N_9O_{21}$	7	10(−3)
151	1,1,1,7,7,7-Hexanitroheptanone-4	$C_7H_8N_6O_{13}$	34	35(−1)
152	Methylene-bis-(trinitroethyl)-carbamate	$C_7H_8N_8O_{16}$	27	12(15)
153	2,2-Dinitropropyltrinitrobutyrate	$C_7H_9N_5O_{12}$	151	89(62)
154	2,2,2-Trinitroethyl-4,4-dinitrovalerate	$C_7H_9N_5O_{12}$	70	89(−19)
155	Bis-(2,2-dinitropropyl)-carbonate	$C_7H_{10}N_4O_{11}$	300	191(109)
156	2,2-Dinitropropyl-4,4,4-trinitrobutyramide	$C_7H_{10}N_6O_{11}$	72	73(−1)
157	Bis-(trinitropropyl)-urea	$C_7H_{10}N_8O_{13}$	23	23(0)
158	Bis-(1,1,1-trinitro-2-propy)-urea	$C_7H_{10}N_8O_{13}$	19	23(−4)
159	Bis-(trinitroethyl)-fumarate	$C_8H_6N_6O_{16}$	14	53(−39)
160	Trinitroethyl-bis-(trinitroethoxy)-acetate	$C_8H_7N_9O_{22}$	6	9(−3)
161	4,4,4-Trinitrobutyric anhydride	$C_8H_8N_6O_{15}$	30	40(−10)
162	Bis-(2,2,2-trinitroethyl)-succinate	$C_8H_8N_6O_{16}$	30	41(−11)
163	Bis-(2,2-dinitropropyl)-oxalate	$C_8H_{10}N_4O_{12}$	227	183(44)
164	N,N′-Bis-(3,3,3-trinitropropyl)-oxamide	$C_8H_{10}N_8O_{14}$	45	29(16)
165	2,2,2-Trinitroethyl-4,4-dinitrohexanoate	$C_8H_{11}N_5O_{12}$	138	146(−8)
166	2,2-Dinitrobutyl-4,4,4-trinitrobutramide	$C_8H_{11}N_5O_{12}$	101	146(−45)
167	2,2-Dinitropropyl-4,4-dinitrovalerate	$C_8H_{12}N_4O_{10}$	320	299(21)
168	Nitroisobutyl-4,4,4-trinitrobutrate	$C_8H_{12}N_4O_{10}$	279	299(−20)
169	Tetrakis-(2,2,2-trinitroethyl)-orthocarbonate	$C_9H_8N_{12}O_{28}$	7	10(−3)
170	Methylene-bis-(4,4,4-trinitrobutramide)	$C_9H_{12}N_8O_{14}$	113	58(55)
171	Ethylene-bis-(4,4,4-trinitrobutrate)	$C_{10}H_{12}N_6O_{16}$	120	121(−1)
172	N,N-Bis-(2,2-dinitropropyl)-4,4,4-trinitrobutramide	$C_{10}H_{14}N_8O_{15}$	72	87(−15)
173	Bis-(2,2,2-trinitroethyl)-4,4-dinitroheptanedioate	$C_{11}H_{12}N_8O_{20}$	68	61(7)
174	2,2-Dinitropropane-1,3-diol-(4,4,4-trinitrobutrate)	$C_{11}H_{12}N_8O_{20}$	50	61(−11)
175	Bis-(2,2,2-trinitroethyl)-4,4,6,6,8,8-hexanitro-undecanedioate	$C_{15}H_{16}N_{12}O_{28}$	32	46(−14)
176	N,N′-Dinitromethanediamine	$CH_4N_4O_4$	13	9(4)
177	N-Nitro-N-methyl-formamide	$C_2H_4N_2O_3$	320	226(94)
178	N,N′-Dinitro-1,2-ethanediamine	$C_2H_6N_4O_4$	34	15(19)
179	Methyl-2,2,2-trinitroethylnitramine	$C_3H_5N_5O_8$	9	10(−1)
180	Trinitroethylnitrguanidine	$C_3H_5N_7O_8$	15	19(−4)
181	Cyclotrimethylenetrinitramine	$C_3H_6N_6O_6$	26	31(−5)
182	N-Methyl-N,N′-dinitro-1,2,3-ethanediamine	$C_3H_8N_4O_4$	114	125(−11)
183	Trinitroethylcyanomethyl nitramine	$C_4H_4N_6O_8$	11	25(−14)
184	Bis-(2,2,2-trinitroethyl)-nitramine	$C_4H_4N_8O_{14}$	5	1(4)
185	N-Methyl-N-nitro-(trinitroethyl)-carbamate	$C_4H_5N_5O_{10}$	17	10(7)
186	N,N′-Dimethyl-N,N′-dinitrooxamide	$C_4H_6N_4O_6$	79	93(−14)
187	N-Nitro-N-(trinitroethyl)-glycinamide	$C_4H_6N_6O_9$	17	5(12)
188	Cyclotetramethylenetetranitramine	$C_4H_8N_8O_8$	29	31(−2)
189	N,N′-Dinitro-N-[2-(nitroamino)ethyl]-1,2-ethanediamine	$C_4H_{10}N_6O_6$	39	49(−10)
190	1,3,3,5,5-pentanitro piperidine	$C_5H_6N_6O_{10}$	14	17(−3)
191	2,2,2-trinitroethyl-3′,3′,3′-trinitroethylnitramine	$C_5H_6N_8O_{14}$	6	10(−4)
192	N,N′-Bis-2,2,2-trinitroethyl-N,N′-dinitromethanediamine	$C_5H_6N_{10}O_{16}$	5	10(−5)
193	Trinitroethyl-N-ethyl-N-nitro-carbamate	$C_5H_7N_5O_{10}$	19	26(−7)
194	Tinitroethyl-2-methoxy-ethylnitramine	$C_5H_9N_5O_9$	42	30(12)
195	N-methyl-N′-trinitroethyl-N,N′-dinitro-1,2-ethanediamine	$C_5H_9N_7O_{10}$	11	21(−10)
196	N,N′-3,3-tetranitro-1,5-pentanediamine	$C_5H_{10}N_6O_8$	35	23(12)
197	N-nitro-N-(3,3,3-trinitropropyl)-2,2,2-trinitroethyl carbamate	$C_6H_6N_8O_{16}$	9	11(−2)
198	2,2,2-trinitroethyl-N-(2,2,2-trinitroethyl)-nitramino acetate	$C_6H_6N_8O_{16}$	9	11(−2)

Table 2. (cont.)

No.	Compound	Formula	H_{50} (exp.)[a] (cm)	H_{50} (pred.)[b] (cm)
199	2,2,2-trinitroethyl-4-nitrazavalerate	$C_6H_9N_5O_{10}$	35	114(−79)
200	Trinitropropyl-(2,2-dinitropropyl)-nitramine	$C_6H_9N_7O_{12}$	17	16(1)
201	2′,2′,2′-Trinitroethyl-2,5-dinitrazahexanoate	$C_6H_9N_7O_{12}$	15	30(−15)
202	2,2,2-Trinitroethyl-3,3′-dinitrobuthyl nitramine	$C_6H_9N_7O_{12}$	20	16(4)
203	N-(2,2-Dinitropropyl)-N,2,2-trinitro-1-propanamine	$C_6H_{10}N_6O_{10}$	29	31(−2)
204	1,7-dimethoxy-2,4,6-trinitrazaheptane	$C_6H_{14}N_6O_8$	166	169(−3)
205	N,N′-Dinitro-N,N′-bis[2-(nitroamino)ethyl]-1,2-ethanediamine	$C_6H_{14}N_8O_8$	53	73(−20)
206	Bis-(trinitroethyl)-2,4-dinitrazapentanedioate	$C_7H_6N_{10}O_{20}$	10	24(−14)
207	2,2-dinitropropyl-5,5,5-trinitro-2-nitrazapentanoate	$C_7H_9N_7O_{14}$	16	20(−4)
208	Trinitroethyl-5,5-dinitro-3- nitrazahexanoate	$C_7H_9N_7O_{14}$	25	20(5)
209	2,2,2- Trinitroethyl-2,5,5-trinitro-2-azahexanoate	$C_7H_9N_7O_{14}$	22	20(2)
210	N-nitro-N,N′-bis(trinitropropyl)-urea	$C_7H_9N_9O_{15}$	21	9(12)
211	2,2,2-Trinitroethyl-2,4,6,6-tetranitro-2,4-diazaheptanoate	$C_7H_9N_9O_{16}$	18	3(15)
212	Bis-(2,2,2-trinitroethyl)-3-nitrazaglutarate	$C_8H_8N_8O_{18}$	14	0(14)
213	N,N′-Dinitro-N,N′-bis-3,3,3-trinitropropyl)-oxamide	$C_8H_8N_{10}O_{18}$	9	24(−15)
214	Bis-(trinitroethyl)-2,4,6-trinitraza-heptanedioate	$C_8H_8N_{12}O_{22}$	13	22(−9)
215	2,2,6,9,9-pentanitro-4-oxa-5-oxo-6-azadecane	$C_8H_{12}N_6O_{12}$	47	60(−13)
216	1,1,1,3,6,9,11,11,11-nonanitro-3,6,9-triazaundecane	$C_8H_{12}N_{12}O_{18}$	12	5(7)
217	N-(2-2-Dinitrobutyl)-N-2,2-trinitro-1-butanamine	$C_8H_{14}N_6O_{10}$	80	90(−10)
218	N,N′-Dinitro-N,N′-bis-(3-nitrazabutyl)-oxamide	$C_8H_{14}N_8O_{10}$	90	143(−53)
219	2,2,4,7,9,9,hexanitro-4,7-diazadecane	$C_8H_{14}N_8O_{12}$	72	30(42)
220	N,N′-dinitromethylene-bis-(4,4,4-trinitro)-butyramide	$C_9H_{10}N_{10}O_{18}$	13	21(−8)
221	1,1,1,5,7,10,14,14,14-Nonanitro-3-12-dioxa-4,11-dioxo-5,7,10-triazatetradecane	$C_9H_{10}N_{12}O_{22}$	11	0(11)
222	Bis-(5,5,5-trinitro-3-nitrazapentanoyl)-methylenedinitramine	$C_9H_{10}N_{14}O_{22}$	15	4(11)
223	1,1,1,4,6,6,8,11,11,11-Decanitro-4,8-diazaundecane	$C_9H_{12}N_{12}O_{20}$	11	5(6)
224	1,1,1,3,6,6,9,11,11,11-Decanitro-3,9-diazaundecane	$C_9H_{12}N_{12}O_{20}$	10	5(5)
225	Bis-(2,2,2-trinitroethyl)-4-nitraza-1,7-heptanedioate	$C_{10}H_{12}N_8O_{18}$	29	41(−12)
226	Bis-(2,2,2-trinitroethyl)-3,6-dinitraza-1,8-octanedioate	$C_{10}H_{12}N_{10}O_{20}$	29	17(12)
227	Bis-(trinitroethyl)-2,5,8-trinitraza nonanedioate	$C_{10}H_{12}N_{12}O_{22}$	17	8(9)
228	N,N′-Dinitro-N,N′-bis-(3,3-dinitrobutyl)-oxamide-triazatetradecane	$C_{10}H_{14}N_8O_{14}$	37	51(−14)
229	1,1,1,3,6,9,12,14,14,14-Decanitro-3,6,9,12-tetrazatetradecane	$C_{10}H_{16}N_{14}O_{20}$	19	18(1)
230	Bis-(trinitroethyl)-5,5-dinitro-2,8-dinitraza-nonanedioate	$C_{11}H_{12}N_{12}O_{24}$	12	7(5)
231	2,2,4,7,7,10,12,12-Octanitro-4,10-diazatridecane	$C_{11}H_{18}N_{10}O_{16}$	44	36(8)
232	2,2,5,7,7,9,12,12-octanitro-5,9-diazatridecane	$C_{11}H_{18}N_{10}O_{16}$	37	36(1)
233	1,4-Bis-(5,5,5-trinitro-2-nitrazapentanoate)-2-butyne	$C_{12}H_{12}N_{10}O_{20}$	16	44(−28)
234	1,1,1,18,18,18-Hexanitro-3,16-dioxa-4,15-dioxo-5,8,11,14-tetranitrazaoctadecane	$C_{12}H_{16}N_{14}O_{24}$	19	17(2)
235	1,1,1,3,6,6,8,10,,10,13,15,15,15-tridecanitro-3,8,13-triazapentadecane	$C_{12}H_{16}N_{16}O_{26}$	23	7(16)
236	2,2-Dinitropropanediol-bis-(5,5-dinitro-2-nitraza-hexanoate)	$C_{13}H_{18}N_{10}O_{20}$	138	113(25)
237	1,2,3-Propanetriol trinitrate	$C_3H_5N_3O_9$	20	10(10)
238	N-(2,2,2-trinitroethyl)-nitraminoethyl nitrate	$C_4H_6N_6O_{11}$	7	10(−3)
239	2,2-Bis-(nitroxymethyl)-1,3-propanediol dinitrate	$C_5H_8N_4O_{12}$	13	52(−39)
240	3-[N-(2,2,2-trinitroethyl)-nitramino]-propyl nitrate	$C_5H_8N_6O_{11}$	12	8(4)
241	3,5,5-Trinitro-3-azahexyl nitrate	$C_5H_9N_5O_9$	21	59(−38)
242	1,9-Dinitrato-2,4,6,8-tetranitrazanonane	$C_5H_{10}N_{10}O_{14}$	10	10(0)
243	4,4,8,8-Tetranitro-1,11-dinitrato-6-nitraza undecane	$C_{10}H_{16}N_8O_{16}$	87	63(24)
244	3-nitro-1,2,4-triazole	$C_2H_2N_4O_2$	320	301(19)
245	3-Nitro-1,2,4-triazole-5-one	$C_2H_2N_4O_3$	291	236(55)
246	Ammonium 3-nitro-1,2,4-triazolate	$C_2H_5N_5O_2$	320	350(−30)
247	Ammonium 3,5-dinitro-1,2,4-triazolate	$C_2H_4N_6O_4$	110	112(−2)
248	4-Methyl-3,5-dinitro-1,2,4-triazole	$C_3H_3N_5O_4$	155	179(−24)
249	5,5′-Dinitro-3,3′-bi-1,2,4-triazole	$C_4H_2N_8O_4$	153	222(−69)
250	4-(2-Nitroethyl)-3,5-dinitro-1,2,4-triazole	$C_4H_4N_6O_6$	35	66(−31)
251	3-Nitro-1-picryl-1,2,4-triazole	$C_8H_3N_7O_8$	320	302(18)
252	1-picryl-1,2,4-triazole	$C_8H_5N_5O_{10}$	68	197(−129)
253	3-picrylamino-1,2,4-triazole	$C_8H_5N_7O_6$	320	255(65)
254	4-picrylamino-1,2,4-triazole	$C_8H_5N_7O_6$	314	302(12)
255	3-Amino-5-picrylamino-1,2,4-triazole	$C_8H_6N_8O_6$	230	266(−36)
256	4-(2,4-Dinitrobenzyl)-3,5-dinitro-1,2,4-triazole	$C_9H_5N_7O_8$	96	229(−133)
257	4-(4-Nitrobenzyl)-3,5-dinitro-1,2,4-triazole	$C_9H_6N_6O_6$	320	328(−8)
258	2-picryl-3-picrylamino-1,2,4-triazole	$C_{14}H_6N_{10}O_{12}$	320	234(6)
259	3,5-Bispicrylamino-1,2,4-triazole	$C_{14}H_7N_{11}O_{12}$	240	222(98)

Table 2. (cont.)

No.	Compound	Formula	H_{50} (exp.)[a] (cm)	H_{50} (pred.)[b] (cm)
260	N,N′-Dipicryl-5,5′-dinitro-3,3′-bi-1,2,4-triazole	$C_{16}H_4N_{14}O_{16}$	138	183(−45)
261	5,5′-Bispicrylamino-3,3′-bi-1,2,4-triazole	$C_{16}H_8N_{14}O_{12}$	320	289(31)
262	4-Nitro-1,2,3-triazole	$C_2H_2N_4O_2$	25	178(−153)
263	Ammonium 4-nitro-1,2,3-triazole	$C_2H_5N_5O_2$	235	235(0)
264	4-Nitro-1-picryl-1,2,3-triazole	$C_8H_3N_7O_8$	9	46(−37)
265	4-Nitro-1-picryl-1,2,3-triazole	$C_8H_3N_7O_8$	67	46(21)
266	1-(3′,5′-dinitrophenyl)-4-nitro-1,2,3-triazole	$C_8H_4N_6O_6$	56	57(−1)
267	1-(3′,4′-dinitrophenyl)-4-nitro-1,2,3-triazole	$C_8H_4N_6O_6$	51	57(−6)
268	1-picryl-1,2,3-triazole	$C_8H_4N_6O_6$	10	57(−47)
269	2-picryl-1,2,3-triazole	$C_8H_4N_6O_6$	200	57(143)
270	1-(3′-Amino-2′,4′,6′-trinitrophenyl)-1,2,3-triazole	$C_8H_5N_7O_6$	31	71(−40)
271	4-Picrylamino-1,2,3-triazole	$C_8H_5N_7O_6$	103	71(32)
272	4,6-Dinitro-1-picryl benzotriazole	$C_{12}H_4N_8O_{10}$	40	64(−24)
273	5,6-Dinitro-1-picryl benzotriazole	$C_{12}H_4N_8O_{10}$	35	64(−29)
274	1-picryl-4-picrylamino-1,2,3-triazole	$C_{14}H_6N_{10}O_{12}$	35	61(−26)
275	2,6-Dipicrylbenzo-[1,2-d:4,5-d′]-bistriazole-4,8-dione	$C_{18}H_4N_{12}O_{14}$	95	48(−47)
276	1,7-Dipicrylbenzo-[1,2-d:4,5-d′]-bistriazole	$C_{18}H_6N_{12}O_{12}$	38	55(−17)
277	1,5-Dipicrylbenzo-[1,2-d:4,5-d′]-bistriazole	$C_{18}H_4N_{12}O_{14}$	40	55(−15)
	RMS deviation (cm)		41	
	RMS-relative (%)		93	

[a] Reported H_{50} values for numbers 1 to 36 were taken from [51] and the other values from [45].
[b] Difference in H_{50} values (in cm) given in parentheses.

Table 3. Comparison of predicted H_{50} of the present work in test set with experimental data as well as five quantum mechanical models [51].

No.	Compound	formula	H_{50} (exp.)[a] (cm)	H_{50} (pred.)[b] (cm)	H_{50} (cm) Model 1	H_{50} (cm) Model 2	H_{50} (cm) Model 3	H_{50} (cm) Model 4	H_{50} (cm) Model 5
1	Tetranitrate pentaerythritol	$C_5H_8N_4O_{12}$	13	13(0)	88(−75)	28(−15)	30(−17)	41(−28)	16(−3)
2	2,4,6,8,10,12-Hexanitro hexaaza isowurtzitane(ε-polymorph)	$C_5H_8N_4O_{12}$	12	49(−37)	45(−33)	16(−4)	29(−17)	29(−17)	3(9)
3	Hexahydro-1,3,5-trinitrotriazine	$C_3H_6N_6O_6$	28	31(−3)	314(−286)	49(−21)	31(3)	39(−11)	22(6)
4	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	$C_4H_8N_8O_8$	32	31(1)	152(−120)	21(11)	31(1)	41(−9)	22(10)
5	N,N′-Dinitro-1,2-ethenediamine	$C_2H_6N_4O_4$	34	15(19)	1066(−1032)	69(−35)	45(−11)	190(−156)	153(−119)
6	2,4,6-Trinitroresorcinol	$C_6H_3N_3O_8$	43	79(−36)	62(−19)	62(−19)	48(5)	113(−70)	106(−63)
7	2,2′,4,4′,6,6′-Hexanitrostilbene	$C_{14}H_6N_6O_{12}$	54	103(−49)	50(4)	33(21)	34(20)	60(−6)	47(7)
8	1,4-Dinitroimidazole	$C_3H_2N_4O_4$	55	84(−29)	80(−25)	227(−172)	262(−207)	36(19)	38(17)
9	2,4,5-Trinitroimidazole	$C_3HN_5O_6$	68	52(16)	22(46)	19(49)	29(39)	30(38)	4(64)
10	2,4-Dinitroimidazole	$C_3H_2N_4O_4$	105	162(−57)	61(44)	34(71)	32(73)	59(46)	41(64)
11	1,1-Diamino-2,2-dinitro ethyl	$C_2H_4N_4O_4$	126	31(95)	262(−136)	320(−194)	40(86)	168(−42)	133(−7)
12	2-Methoxy-1,3,5-trinitrobenzene	$C_7H_5N_3O_7$	192	216(−24)	80(112)	86(106)	98(94)	108(84)	128(64)
13	3-Nitro-1,2,4-triazole-5-one	$C_2H_2N_4O_3$	291	149(142)	193(98)	78(213)	35(256)	668(−377)	296(−5)
14	Nitroguanidine	$CH_4N_4O_2$	320	248(72)	1121(−801)	276(44)	139(181)	5339(−5019)	1800(−1480)
	RMS deviation (cm)			56	364	99	109	1346	398
	RMS-relative (%)			96	882	112	122	447	165

[a] Reported H_{50} values were taken from [51].
[b] Difference in H_{50} values (in cm) given in parentheses.

relationship between both. Our proposed method is superior to that of quantum mechanical procedure in terms of accuracy, generality and simplicity as it requires only the molecular structure of the explosive compound, which is always known. As can be seen, artificial neural networks are able to capture the nonlinearity in the system behavior very

effectively. Moreover, the connection weights and network architecture make predictions possible using a spreadsheet. The new procedure can be applied for calculating impact sensitivities of any $C_aH_bN_cO_d$ explosive and requires only the explosive's composition. Since high percentage errors are generally attributed to 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 explosives of practical importance. As can be seen in Table 3, results predicted by using artificial neural network are comparable with outputs from complicated quantum mechanical computations and the accuracy of prediction is not necessarily enhanced by greater complexity.

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