

# Neural networks study on the correlation between impact sensitivity and molecular structures for nitramine explosives

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**Abstract** In this paper, a back-propagation neural network has been utilized to study on the correlation between impact sensitivity and molecular properties of 33 nitramine molecules. By using density functional theory method B3P86/6-31G\*\*, all the molecular properties have been calculated. Eight different sets of molecular properties, including (HOMO – LUMO)\*BDE,  $E$ , BDE/ $E$ , HOMO – LUMO, BDE\* $\mu$ ,  $R^2$ ,  $\Delta E$ , and BDE, have been used to train and test the network. Based on the test results, the correlation order between the molecular properties and impact sensitivity has been achieved. The correlation order shows that the input set with the descriptor  $\Delta E$  (atomization energy) can obtain better results than any other descriptor for nitramines, which surely accounts for a comparatively stronger correlation between  $\Delta E$  (atomization energy) and impact sensitivity for nitramines we have studied in this work.

**Keywords** Neural networks · Impact sensitivity · Back-propagation algorithm · Nitramines · Molecular descriptors

## Introduction

The study on the correlation between impact sensitivity of energetic materials and molecular structures has recently been an ongoing area of research in explosive theory [1]. The so-

called impact sensitivity  $h_{50\%}$  is measured experimentally by drop weight impact test, where a height of 50% probability in causing an explosion is measured when hit by a hammer with a standard weight [2, 3]. Since storage, synthesis, and application of energetic materials are significantly affected by impact or shock sensitivity, the researches about the impact sensitivity is of primary importance. Once we get the ability to predict potential explosives using computational methods, it will provide significant cost savings, increase the safety of storage and testing of these compounds, and provide for greater control of the performance of these explosives [4]. Presently, the usage of quantum mechanical methods as a predictive tool for assessing relationships between molecular properties of various explosive molecules and their impact sensitivities has been suggested in several previous works. Correlations between impact sensitivity and chemical composition reported earlier by Kamlet and Adolph were probably the most widely applied in the area of energetic materials research [5]. These demonstrated that for families of high-energy molecules with similar decomposition mechanisms, there were approximately linear relationships between  $\log h_{50\%}$  and  $OB_{100}$ , the latter was a measure of “oxygen balance”; MNDO/3 molecular orbital method was used by Owens [6] to calculate the energy for bond rupture for a number of energetic molecules and the results showed that the weakest bond was generally that between the  $NO_2$  and the remainder of the molecule. In addition, his calculation results indicated a correlation between the magnitude of the energy barrier and the susceptibility to detonation; Politzer [7] investigated shock-sensitivity relationships for nitramines and nitroaliphatics, and showed that shock sensitivity was related to the strengths of all the N– $NO_2$  and C– $NO_2$  bonds, taken in conjunction with overall molecular size; Rice and co-workers [8, 9] pointed out that for nitroaromatic molecules there was a correlation between the

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bond dissociation energy of the weakest bond and sensitivity. Moreover, they investigated the relation between impact sensitivity and charge distribution in energetic molecules; Xiao and co-workers [10–12] once proposed a principle of the smallest bond order to identify the relative magnitudes of impact sensitivity of most energetic compounds. For polynitroaromatic series, Jinshan and Gang [1] showed that the Mulliken bond order of C–NO<sub>2</sub> linkage correlated well with the observed values of  $h_{50\%}$ ; Zeman found a logarithmic relationship between the drop energy  $E_{dr}$  and heats of fusion for 33 polynitro compounds [13]. The correlation between impact sensitivity and approximated heats of detonation of several nitramines was examined by Edwards et al. [4]. Besides, many other properties have been found to correlate with impact sensitivities. These properties include molecular electronegativities [14, 15], vibrational states [16, 17], molecular weights and detonation gas concentrations [18], parameters related to oxidation numbers [19], partial atomic charges [15, 20–24], heats of reaction [25, 26], heats of explosion [27], bond orders [28, 29], and activation energies [27–31]. Although works listed above succeeded in finding a certain kind of correlations between some of the specific molecular properties and the impact sensitivity, many of the correlations almost existed in a certain type of explosive and the number of explosives in each type was usually small. In addition, most of the works simply examined the correlation between one or two molecular properties and impact sensitivity of explosive compounds. Consequently, in order to make a further study on the correlation between impact sensitivity and molecular properties, investigations should be carried out on how molecular properties affect impact sensitivity for the same type of energetic materials with similar molecular structure. In the present work, DFT method B3P86/6-31G\*\* is adopted to calculate molecular properties of 33 nitramine explosives, and artificial neural networks method is utilized to research the correlation order between different molecular properties and impact sensitivity.

The neural network is a nonlinear function of many parameters that maps particular inputs (in our case, molecular properties) to an output (in our case, impact sensitivity). The network is made up of simple, yet highly connected, processing elements called nodes [32]. They are computer-based emulations of the brain's information-processing capability [3]. Neural networks have been applied to various engineering problems, such as robotics, pattern recognition, speech, etc. [33]. In addition, the use of neural network methods has grown constantly in a variety of applications in chemistry and physics since their first utilization for the prediction of protein secondary structure. For example, neural networks have been used to calculate the ground-state eigenenergy of two-dimensional harmonic oscillators [34], to solve nonhomogeneous ordinary and partial differential equations [35], and to obtain the electronic correlation energy for atoms and

diatomic molecules [36]. But for the explosive engineering, there exist few reports about the impact sensitivity based on neural networks method, although Nefati [3] and Cho et al. [37] predicted the impact sensitivity of various types of explosive molecules via neural networks. However, they both provided better impact sensitivity values by employing dozens of compositional and topological descriptors, which is not very realistic for explosive synthesis engineering, and which property can correlate with the sensitivity best is still not clear. In the current work, we will choose five fundamental molecular descriptors in each input set so as to examine the sensitivities more conveniently. Since the fundamental molecular properties were easier to calculate, correlation study should be used to identify fundamental molecular properties that indicate sensitivity best. In addition, their works did not include the correlation order between impact sensitivity and molecular properties, which will be studied in the following part of this paper.

Energetic secondary nitramines are currently a subject of increasing interest in high-energy materials research. Of particular importance are efforts aimed at gaining insight into how molecular features of nitramines influence their impact sensitivities.

In this paper, we will utilize the back-propagation neural network (BP) to analyze the correlation between impact sensitivity of nitramines and molecular properties. In particular, the correlation order between various molecular properties and impact sensitivity will also be examined.

## Theoretical methods

### Calculation method

Thirty-three nitramine molecules as shown in Table 1 were investigated in this paper. All the experimental impact sensitivity values were taken from [38]. In this work, by using Gaussian 98 hybrid DFT B3P86 method, the Becke-style three-parameter density functional theory [39] with the Perdew's 86 (P86) [40] in combination with the basis set 6-31G\*\* [41], the geometry was optimized and then the molecular structures were calculated. The calculated molecular properties included the sum of electronic and zero-point energy ( $E$ ), zero-point vibration energy (ZPE), dipole moment ( $\mu$ ), electronic spatial extent ( $R^2$ ), highest occupied molecular orbital (HOMO), and lowest unoccupied molecular orbital (LUMO). Furthermore, the atomization energy of various explosive molecules ( $\Delta E$ ) and the bond dissociation energy of the weakest X–NO<sub>2</sub> bond (BDE) were also calculated in this paper.

One can expect that the properties listed above examined for correlations contain many "obvious" choices and may be already well described in previous works. That is true when

**Table 1** Thirty-three nitriamine molecular formulas and our final calculated values ( $h_{50\%}$ , cm) using set 6 and set 1 along with experimental values

Serial no	Formula	Compound names	Experimental $h_{50\%}$ [46]	Our results <sup>a</sup>	Our results <sup>b</sup>
1	CH <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	Nitroguanidine	59	54	35
2	CH <sub>4</sub> N <sub>4</sub> O <sub>4</sub>	<i>N,N'</i> -Dinitro-methanediamine	13	11	6
3	C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>	<i>N</i> -Nitro- <i>N</i> -methyl-formamide	320	314	278
4	C <sub>2</sub> H <sub>6</sub> N <sub>4</sub> O <sub>4</sub>	<i>N,N'</i> -Dinitro-1,2-ethanediamine	34	43	29
5	C <sub>3</sub> H <sub>5</sub> N <sub>7</sub> O <sub>8</sub>	Trinitroethyl-nitroguanidine	15	15	32
6	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	Cyclotrimethylene-trinitramine	26	23	41
7	C <sub>3</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>	<i>N</i> -Methyl- <i>N,N'</i> -dinitro-1-2-ethanediamine	114	110	138
8	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>8</sub>	Trinitroethyl-cyanomethylnitramine	11	12	24
9	C <sub>4</sub> H <sub>5</sub> N <sub>5</sub> O <sub>10</sub>	<i>N</i> -Methyl- <i>N</i> -nitro-(trinitroethyl)-carbamate	17	18	26
10	C <sub>4</sub> H <sub>6</sub> N <sub>6</sub> O <sub>9</sub>	<i>N</i> -Nitro- <i>N</i> -(trinitro-ethyl)-glycinamide	17	13	29
11	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>6</sub>	<i>N,N'</i> -Dimethyl- <i>N,N'</i> -dinitrooxamide	79	85	73
12	C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	Cyclotetramethylene-tetranitramine	29	24	49
13	C <sub>4</sub> H <sub>10</sub> N <sub>6</sub> O <sub>6</sub>	<i>N,N'</i> -Dinitro- <i>N</i> -[2-(nitroamino)ethyl]-1,2-ethanediamine	39	35	57
14	C <sub>5</sub> H <sub>6</sub> N <sub>6</sub> O <sub>10</sub>	1,3,3,5,5-Pentanitro-piperidine	14	17	26
15	C <sub>5</sub> H <sub>7</sub> N <sub>5</sub> O <sub>10</sub>	Trinitroethyl- <i>N</i> -ethyl- <i>N</i> -nitro-carbamate	19	23	26
16	C <sub>5</sub> H <sub>9</sub> N <sub>5</sub> O <sub>9</sub>	Trinitroethyl-2-methoxy-ethylnitramine	42	48	46
17	C <sub>5</sub> H <sub>10</sub> N <sub>6</sub> O <sub>8</sub>	<i>N,N'</i> -3,3-Tetranitro-1,5-pentanediamine	35	37	62
18	C <sub>6</sub> H <sub>9</sub> N <sub>5</sub> O <sub>10</sub>	2,2,2-Trinitroethyl-4-nitrazavalerate	35	35	49
19	C <sub>6</sub> H <sub>9</sub> N <sub>5</sub> O <sub>10</sub>	Trinitropropyl-(2,2-dinitropropyl)-nitramine	17	16	9
20	C <sub>6</sub> H <sub>9</sub> N <sub>7</sub> O <sub>12</sub>	2',2',2'-Trinitroethyl-2-5-dinitrazahexanoate	15	14	30
21	C <sub>6</sub> H <sub>9</sub> N <sub>7</sub> O <sub>12</sub>	2,2,2-Trinitroethyl-3,3-dinitrobutyl-nitramine	20	23	52
22	C <sub>6</sub> H <sub>10</sub> N <sub>6</sub> O <sub>10</sub>	<i>N</i> -(2,2-Dinitropropyl)- <i>N</i> ,2,2-trinitro-1-propanamine	29	31	38
23	C <sub>6</sub> H <sub>14</sub> N <sub>6</sub> O <sub>8</sub>	1,7-Dimethoxy-2,4,6-trinitrazaheptane	166	165	147
24	C <sub>6</sub> H <sub>14</sub> N <sub>8</sub> O <sub>8</sub>	<i>N,N'</i> -Dinitro- <i>N,N'</i> -bis[2-(nitroamino)ethyl]-1,2-ethanediamine	53	57	73
25	C <sub>7</sub> H <sub>9</sub> N <sub>7</sub> O <sub>14</sub>	2,2-Dinitropropyl-5,5,5-nitrazapentanoate	16	25	32
26	C <sub>7</sub> H <sub>9</sub> N <sub>7</sub> O <sub>14</sub>	Trinitroethyl-5,5-dinitro-3-nitrazahexanoate	25	21	38
27	C <sub>7</sub> H <sub>9</sub> N <sub>7</sub> O <sub>14</sub>	2,2,2-Trinitroethyl-2,5,5-trinitro-2-azahexanoate	22	32	35
28	C <sub>7</sub> H <sub>9</sub> N <sub>7</sub> O <sub>14</sub>	<i>N</i> -Nitro- <i>N,N'</i> -bis(trinitropropyl)-urea	21	24	37
29	C <sub>7</sub> H <sub>9</sub> N <sub>9</sub> O <sub>16</sub>	2,2,2-Trinitroethyl-2,4,6,6-tetranitro-2,4-diazaheptanoate	18	22	40
30	C <sub>8</sub> H <sub>12</sub> N <sub>6</sub> O <sub>12</sub>	2,2,6,9,9-Pentanitro-4-oxa-5-oxo-6-azadecane	47	40	76
31	C <sub>8</sub> H <sub>14</sub> N <sub>6</sub> O <sub>10</sub>	<i>N</i> -(2,2-Dinitrobutyl)- <i>N</i> ,2,2-trinitro-1-butanamine	80	82	63
32	C <sub>8</sub> H <sub>14</sub> N <sub>8</sub> O <sub>10</sub>	<i>N,N'</i> -Dinitro- <i>N,N'</i> -bis-(3-nitrazabutyl)-oxamide	90	84	48
33	C <sub>8</sub> H <sub>14</sub> N <sub>8</sub> O <sub>12</sub>	2,2,4,7,9,9,Hexanitro-4,7-diazadecane	72	69	85

<sup>a</sup>Impact sensitivity values obtained by employing set 6 containing  $\Delta E$ .

<sup>b</sup>Impact sensitivity values obtained by employing set 1 containing (HOMO – LUMO)\*BDE.

only one or two molecular properties are examined. But until recently, the correlation order of different molecular properties with impact sensitivity has not been studied for the same type of energetic materials with similar molecular structure, and which property correlates with sensitivity best is still not known when different properties are considered. Here, we would like to present a detailed study on the correlation between different molecular properties and impact sensitivity for nitramines.

#### Back-propagation neural network

In the field of structure–activity or structure–property relationships, the back-propagation neural networks, particularly

the three-layer networks, have gained wide acceptance [3]. So a fully connected three-layer architecture, which had an input layer, a hidden layer, and an output layer, was adopted in our neural network.

A back-propagation neural network, which was first developed by Rumelhart and McClelland [42], “learns” by repeatedly passing data through neurons and adjusting their weights and biases to minimize the mean-squared error (MSE),  $\sum (t_i - o_i)^2/n$  ( $t_i$  is a training observation and  $n$  is the total number of input vectors), until the output ( $o_i$ ) predicted by network matches the target ( $t_i$ ) or given property point values.

The neural network can be trained to perform a particular task using a variety of learning algorithms. In this paper, we chose BP algorithm implementing Levenberg–Marquardt

variation for the network, whose training speed was much faster than that of a gradient descent algorithm [43].

By using BP neural network, emphasis was primarily laid on finding out the molecular descriptor, which had the strongest correlation with impact sensitivity of nitramines. Thus, impact sensitivity  $h_{50\%}$  was an obvious choice of the only output neuron. Similarly, selecting the proper molecular descriptors of nitramine molecules, which were to be used as the input neurons of the neural network, was also our focus. After a preliminary evolutionary multiple linear regression treatment,  $BDE/E$ ,  $BDE^*\mu$ ,  $HOMO - LUMO$ ,  $\mu$ ,  $R^2$ ,  $BDE$ ,  $\Delta E$ ,  $(HOMO - LUMO)*BDE$  and the number of C, H, N, O atoms in each CHNO nitramine molecule, which indicated the value of bond dissociation energy divided by total energy, bond dissociation energy multiplied by dipole moment, energy gap, electronic spatial extent, bond dissociation energy, atomization energy, and energy gap multiplied by bond dissociation energy, respectively, were chosen as input descriptors. In order to find out the correlation order between molecular descriptors and impact sensitivity of nitramine molecules, the descriptors mentioned above were divided into eight different sets, each were combined with the number of C, H, N, O atoms comprising each CHNO nitramine molecule. In this case, eight different input sets, with the number of C, H, N, O atoms being the common descriptors in each set, were constructed, as summarized in Table 2.

Usually, the difficulty in finding optimum neural-network architecture resided in deciding on the number of hidden layers and the number of neurons in them. By trial and error, we found that only one hidden layer containing two neurons yielded better overall results than those with more neurons in hidden layers despite the fact that these latter networks could give slightly better fitting of the data set. Therefore, the 5-2-1 structure, which was 5 neurons in input layer, 2 neurons in hidden layer, and 1 neuron in output layer, was adopted for our neural network as depicted in Fig. 1.

During training and test process, we divided 33 nitramine molecules into two groups, a training group and a test group, respectively. The training group was used to help the net

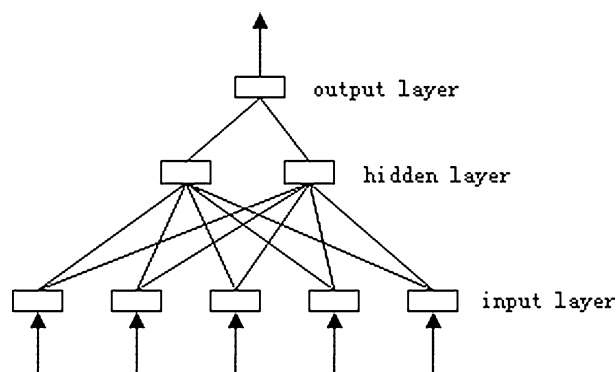


Fig. 1 5-2-1 BP network structure

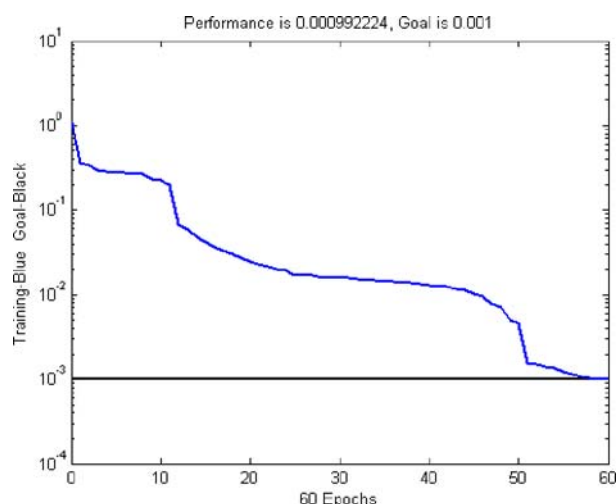
learn the relationship between the given input vectors and the target output vector. Meanwhile, the test set consisting of a few compounds, some of which may be dissimilar to the training group, were chosen to validate the network's generalization ability. In order to accelerate the convergent speed, input groups must be normalized. The normalized formula is

$$x'_i = (x_i - u) / s_d \quad (1)$$

where  $x'_i$  is the data after normalization,  $x_i$  is the original data,  $u$  and  $s_d$  are respectively the average value and standard error of the original data [44]. Now, various types of threshold functions are used in neural networks [45], the most common being the sigmoid function, which is incorporated as a transfer function in the MATLAB Neural Network Toolbox 3.0, installed in a PC computer. In this paper, the log sigmoid transfer function,  $\log(1/1 + e - z)$  was used to calculate the outputs of the neurons in hidden layer and output layer. The training parameters were generated randomly. The learning rate was optimized by trial and error and the best value obtained was 0.05. The reasonable output error was 0.001. The neural network was trained for 2000 epochs (using incremental updating or randomization of the training data order to avoid local minima), which were required to reach a maximum error of 0.001. In Fig. 2, the maximum error of the network could be observed as a function of the

**Table 2** Twelve molecular descriptors and eight different input sets calculated for this study

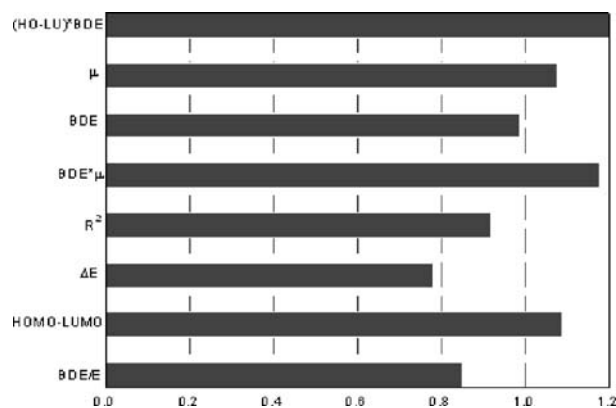
Number	Descriptors	Number	Descriptors
1	Number of C atoms	7	BDE
2	Number of H atoms	8	$BDE^*\mu$
3	Number of N atoms	9	$R^2$
4	Number of O atoms	10	$\Delta E$
5	$(HOMO - LUMO)*BDE$	11	$HOMO - LUMO$
6	$\mu$	12	$BDE/E$
Set 1	Descriptors 1–5	Set 5	Descriptors 1–4, 9
Set 2	Descriptors 1–4, 6	Set 6	Descriptors 12, 3, 4, 10
Set 3	Descriptors 1–4, 7	Set 7	Descriptors 1–4, 11
Set 4	Descriptors 1–4, 8	Set 8	Descriptors 1–4, 12



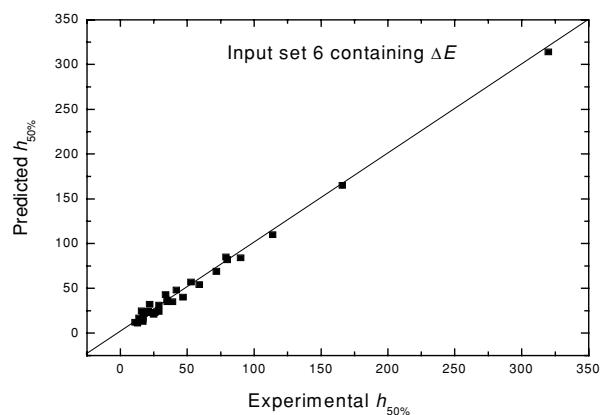
**Fig. 2** The curve of generation ability of the network

number of propagation cycles during the training process. As can be seen, the estimate of the network accuracy was asymptotically decreasing functions. After about 60 cycles, the network converged to a maximum error of 0.00099. Further training could not improve the performance of the network, and at this point training was stopped.

After training process, a few more nitramine molecules, which belonged or did not belong to the input groups, were chosen as test group to validate the generation ability of the network. The reasoning for this specific construction was to allow the test group to contain molecules which were dissimilar to the training group, so that the test and prediction results would exhibit distinct outliers. The test procedure was repeated five times starting from different initial random sets of weights, a technique known to weaken the detrimental effects of local minima on the error surface [46], and the mean-square errors were calculated, as shown in Fig. 3. The mean values, which were obtained by employing set 6, were used as the final values presented in Table 1. Meanwhile, the predicted impact sensitivity values of nitramines calculated by employing set 1 were also listed in Table 1 for compari-



**Fig. 3** Comparison of mean-squared error for eight input sets

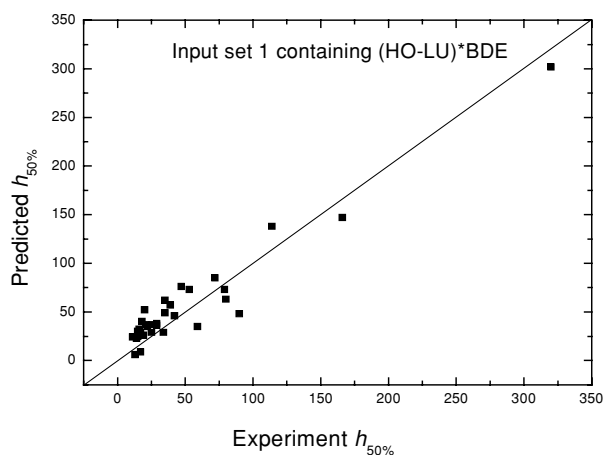


**Fig. 4** Predicted vs. experimental  $h_{50\%}$  values obtained by employing set 6 containing  $\Delta E$

son. Two plots of predicted versus experimental  $h_{50\%}$  values obtained by employing input set 6 and set 1 are depicted in Figs. 4 and 5 to illustrate our conclusion more intuitively.

## Results and discussion

As shown in Fig. 3, MSE values were in the range from 0.782 to 1.200. The smallest MSE value was from the set 6 with  $\Delta E$ , and the biggest MSE value was from the set 1 including (HOMO – LUMO)\*BDE. It indicated that with the same network architecture and training parameters, molecular descriptor  $\Delta E$  had the strongest correlation while (HOMO – LUMO)\*BDE had the slightest correlation with impact sensitivity of the nitramines studied in this work. It is noteworthy that the correlation order studied here was in fact between input sets and impact sensitivity. Since cross-correlation of descriptors in each input set was very slight and each set had four common descriptors, the difference of MSE values in training and test process can be thought



**Fig. 5** Predicted vs. experimental  $h_{50\%}$  values obtained by employing set 1 containing (HOMO – LUMO)\*BDE

mainly coming from very different descriptor in each input set. Thus, we considered the correlation order was mainly decided by the very different descriptor in each set.

Two plots of predicted versus experimental  $h_{50\%}$  values obtained by employing set 6 and set 1 are displayed in Figs. 4 and 5, respectively. Solid lines indicate perfect agreement between experiment and prediction. As shown in Fig. 5, we could see that the predicted values in set 1, in which the molecular descriptor (HOMO – LUMO)\*BDE was included, were mostly larger than the experimental data. Nevertheless, in Fig. 4, the predicted values in set 6, in which  $\Delta E$  was contained, were in excellent agreement with the experimental values. It clearly indicated that  $\Delta E$  had the strongest correlation with impact sensitivity while (HOMO – LUMO)\*BDE had the slightest correlation with impact sensitivity. Predicted values in other six sets were all worse than set 6, but better than set 1.

In quantum chemistry, atomization energy ( $\Delta E$ ) was defined as the difference between molecular energy and the sum of energies of atoms comprising the molecule. For instance such as  $\text{CH}_4\text{N}_4\text{O}_2$ ,

$$\Delta E(\text{CH}_4\text{N}_4\text{O}_2) = E(\text{C}) + 4E(\text{H}) + 4E(\text{N}) + 2E(\text{O}) - E(\text{CH}_4\text{N}_4\text{O}_2) \quad (2)$$

For nitramine explosives, whose structures were mainly made up of carbon chains, the molecular descriptor  $\Delta E$  had the strongest correlation with impact sensitivities. This conclusion was in agreement with Edward et al.'s work [4].

BDE here was defined as the difference between the zero-point-corrected energy of parent nitramine molecule and that of the products of the unimolecular dissociation in which an  $\text{NO}_2$  group was removed. For example, for  $\text{CH}_4\text{N}_4\text{O}_2$ , the BDE was

$$\text{BDE}(\text{CH}_4\text{N}_4\text{O}_2) = [E(\text{CH}_4\text{N}_3) + E(\text{NO}_2)] - E(\text{CH}_4\text{N}_4\text{O}_2) \quad (3)$$

It was noteworthy that for nitramines studied in this work, the breaking of the  $\text{R}-\text{NO}_2$  may be the rate-controlling step in the initiation of detonation, which again supported the Owens' conclusion [6]. Based on chemical reaction kinetics, Arrhenius equation showed that the reaction rate constant depended on the ratio of activation barrier to temperature, so the activation energy may be a key factor in impact initiation and sensitivity of a material. As  $\text{BDE}/E$  had a certain relationship with activation energy, a strong correlation might exist between impact sensitivity and  $\text{BDE}/E$ , which indicated that bond dissociation energy in unit molecular energy. In this paper, descriptor  $\text{BDE}/E$  had the second strongest correlation with impact sensitivity of nitramines, with MSE value 0.833.

As depicted in Fig. 3, the correlation order after  $\Delta E$  and  $\text{BDE}/E$  was as follows:  $R^2$ , BDE,  $\mu$ ,  $\text{BDE}^*\mu$ , HOMO – LUMO, and (HOMO – LUMO)\*BDE. For the last one, the difference between LUMO and HOMO was defined as electronic transition level, which had influence on molecular properties. The lower the HOMO was, the larger was the molecular ionization energy. LUMO was related to molecular affinity, the smaller it was, the more the energy of system decreased when electrons came into the orbital. (HOMO – LUMO)\*BDE and HOMO – LUMO had the weakest correlation with impact sensitivity, which indicated that the initial process of detonation correlated slightly with electronic excitation for nitramines we studied.

## Conclusion

In this paper, by using DFT B3P86/6-31G\*\*method, the electronic structures of 33 nitramine molecules were calculated. Based on the calculated molecular properties, we performed BP neural network to study on the correlation between impact sensitivity of nitramine explosives and molecular structures. Eight different input sets were constructed to train the network, and a few more molecules were chosen to test the generation ability of the network. Best results were obtained by employing set 6, which contained the molecular descriptor  $\Delta E$ . The correlation order between impact sensitivity and the descriptors was obtained as follows:  $\Delta E$ ,  $\text{BDE}/E$ ,  $R^2$ , BDE,  $\mu$ ,  $\text{BDE}^*\mu$ , HOMO – LUMO, and (HOMO – LUMO)\*BDE. It demonstrates that the atomization energy  $\Delta E$  is the best index of impact sensitivity for nitramine explosives, and  $\text{BDE}/E$  the second. Whether this conclusion is general for other chemical families needs to be further studied.

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