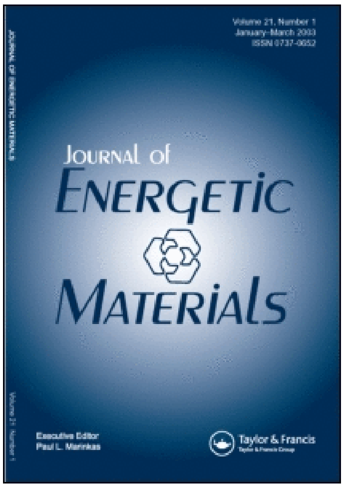

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There has been considerable interest in predicting the stabilities of energetic materials to improve safety during manufacture, handling, storage, and transportation. Although a variety of experimental techniques are available to test the properties of energetic materials, computational screening techniques can harness the convenience of modern computers to reduce the cost of destructive tests.

In this paper quantitative structure–property relationships (QSPRs) based on quantum mechanical calculations were employed to correlate the measured impact sensitivities from shock or impact tests with molecular properties. Molecular descriptors were evaluated using both the Hartree-Fock method with a STO-3G basis set and the semiempirical method PM3. Equations that correlate impact sensitivities to the energy of lowest unoccupied molecular orbital (ε_{LUMO}), energy of highest occupied

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molecular orbital (ε_{HOMO}), midpoint potential (MPP), ionization potential (IP), dipole moment (DM), and total energy (E) of the molecules were developed.

Keywords: impact sensitivity, molecular orbital calculations, QSPR, molecular descriptors

Introduction

Energetic materials such as propellants, pyrotechnics, fuels, and explosives have many industrial and civic applications. Even though these materials have many uses, they still pose dangers and hazards. Impact and shock sensitivity tests commonly are used to measure the tendency of energetic materials to detonate. Most impact tests apply a force to a sample of energetic material by a standard weight falling from various heights, and the sensitivity is inversely proportional to the 50% impact height (h_{50}), which is the height at which there is a 50% probability of initiating an explosion [1].

Some efforts [1–7] have focused on predicting impact sensitivities of energetic materials based on the molecular structures. Kamlet and Adolph [5] developed an approach to classify the sensitivity of C–H–N–O explosives based on their oxygen balance. The oxygen balance was defined as the number of equivalents of oxidant per hundred grams of explosive to burn all hydrogen to water and all carbon to carbon monoxide, as shown below where nCOO is the number of carboxyl groups:

$$\mathrm{OB}_{100} = \frac{100(2n_{\mathrm{O}} - n_{\mathrm{H}} - 2n_{\mathrm{C}} - 2n_{\mathrm{COO}})}{\text{Molecular Weight}}. \tag{1}$$

They proposed correlations in Equations (2)–(6) based on chemical groups. However, across multiple chemical groups, the regressions do not fit the experimental data well:

$$\text{Nitroaromatic,}\ \log h_{50} = 1.73 - 0.32\mathrm{OB}_{100}, \tag{2}$$

$$\text{Nitroaromatic (alpha CH}_3\text{)},\ \log h_{50} = 1.33 - 0.26\mathrm{OB}_{100}, \tag{3}$$

$$\text{Nitroaliphatic,}\ \log h_{50} = 1.74 - 0.23\mathrm{OB}_{100}, \tag{4}$$

$$\text{Dinitrofluoro,}\ \log h_{50} = 2.14 - 0.30\text{OB}_{100}, \tag{5}$$

$$\text{Nitroamine,}\ \log h_{50} = 1.37 - 0.17\text{OB}_{100}. \tag{6}$$

Murray and Politzer [1,6,8] also have developed correlations that help classify and predict the impact and shock sensitivities of explosives based on their molecular electrostatic potential (V_r). They attempted to correlate impact sensitivities with the maxima of V_r on the molecular surface ($V_{\text{s,max}}$), which is not necessarily the midpoint potential of the longest C–NO_2 bond. The developed relationships between sensitivity and $V_{\text{s,max}}$ provided a strong linear correlation coefficient of 0.986 [8]. They also developed a relationship for nitroamines between shock sensitivities and the quantity $(n/M)R_{\text{ave}}$ where n is the number of N–NO_2 bonds, M is the molecular weight, and R_{ave} is the average N–N bond distance. They used this correlation with seven molecules and calculated a correlation coefficient of 0.94 [1]. This correlation proves to be a valuable linkage of impact sensitivities to the strength of N–NO_2 bonds.

Methods

In this work, 10 nitroaromatics, five nitroaromatics with alpha CH_3 bonds, and seven nitroaliphatics were selected as a training set to develop relationships between molecular descriptors and the experimental impact sensitivities (50% impact height or h_{50}) gathered from the literature [5]. The Gaussian 98 suite of programs [9] was employed to calculate the molecular electronic structures and properties of the 22 nitrocompounds. The package includes a wide range of ab initio, density-functional, and semiempirical methods for energy, gradient, frequency, and property calculations. In this work, ab initio molecular orbital calculations were carried out at the Hartree–Fock (HF) level using the STO-3G basis set.

Because of the relative complexity of the molecules studied, it requires tremendous CPU time on supercomputers to calculate the electronic structures and properties using ab initio methods with a moderate basis set. Semiempirical theory PM3 [10], however, is computationally efficient, and only a few seconds are required to optimize the structure of a relative large molecule on a Pentium III PC. For this prediction tool to be practical at the industrial level, MOPAC implemented in the ChemOffice program [11] was used in this work to calculate some appropriate quantum chemical descriptors at the PM3 level.

Quantum Chemical Descriptors

The QSPR relationships usually are derived from the multiple linear least squares regression of the experimentally measured property values (Y) against a set of molecular descriptors (X_1, X_2, ...) [12]. A variety of descriptors can be obtained from experimental measurements and theoretical calculations. The empirical descriptors often represent complex and multiple physical interactions, and may be difficult and expensive to obtain. In contrast, theoretical descriptors derived from quantum mechanical or molecular orbital calculations can be obtained from molecular structures. They represent explicit mathematical definitions and have distinct physical interpretations. In this paper, eight quantum mechanical descriptors were evaluated for the correlation with impact sensitivity.

The evaluated descriptors are discussed as follows:

a. Heat of formation: the heat released or absorbed during the formation of a pure substance from its elements. It is an indicator of relative stability of a compound with its elements. Compounds with positive heats of formation are inherently unstable.
b. Total energy of the molecule (E): This is the sum of the total electronic energy of all molecular orbitals and the potential energy among nuclei in a molecule.
c. Energy of highest occupied molecular orbital ($\varepsilon_{\mathrm{HOMO}}$): The HOMO is the occupied orbital with the highest energy. The higher the energy of HOMO, the easier it is for the molecule to donate an electron and therefore relatively more reactive.
d. Energy of lowest unoccupied molecular orbital ($\varepsilon_{\mathrm{LUMO}}$): The LUMO is the lowest ground-state orbital that does not contain at least one electron. The lower the LUMO

energy, the greater the potential for a molecule to accept an electron.

e. Energy difference between a LUMO and a HOMO: Usually a reaction depends on the interaction between the LUMO and HOMO. The reaction can proceed more readily when the energy difference between the two orbitals is small.
f. Ionization energy (IE): The ionization energy is the amount of energy required to detach one electron from a neutral atom or molecule.
g. Bond length of C–NO_2 bond: The length between the carbon atom and the nitrogen atom. In this work, the longest bond is selected as the weakest C–NO_2 bond.
h. Midpoint potential (V_{mid}): The V_{mid} value was taken at the weakest C–NO_2 bond. The equation used to calculate V_{mid} was $V_{\mathrm{mid}} = (Q_c + Q_n)/0.5R$, where Q_c is the charge on the carbon atom, Q_n is the charge on the nitrogen atom, and R is the distance between the atoms. The Mulliken population analysis was used to estimate the atomic partial charges based on the electron density distribution.
i. Dipole moment (DM): The electric dipole moment for a pair of opposite charges is defined as the magnitude of the charge times the distance between them, and the defined direction is toward the positive charge. The DM is a measure of the asymmetry of the molecular charge distribution.

Statistical Analysis

Multiple linear regression was used to model the relationship between impact sensitivity and molecular descriptors. The developed correlations have the form

$$Y = A_0 + A_1X_1 + A_2X_2 + \cdots + A_nX_n,$$

where Y is the dependent variable, X_1 is an independent variable (molecular descriptor), and A_1 is a regression constant. The regression constants were estimated using the least-squares model implemented in an Excel spreadsheet. Statistical analysis was preformed on the combinations of the descriptors to obtain the correlations with the maximum square of correlation coefficient, R^2 (an indicator of how well the model fits the data). The test for significance of regression was conducted based on F-tests to determine if a linear relationship exists between the dependent variable and a set of independent variables at the 95% confidence level. The statistical significance of each independent variable was based on the p-value from a t-statistic evaluation at the 95% confidence level.

Results and Discussions

Correlations Using Ab Initio Method

The molecular descriptors calculated at the HF/STO-3G level of theory are shown in Table 1. Here $\log(h_{50})$ was chosen as the dependent variable because it provided better correlations than h_{50} values. Different combinations of the molecular descriptors were correlated with $\log(h_{50})$, and the ones that showed significant correlations from the t-statistic tests are the energy difference between LUMO and HOMO ($\varepsilon_{\mathrm{LUMO}} - \varepsilon_{\mathrm{HOMO}}$), energy of LUMO ($\varepsilon_{\mathrm{LUMO}}$), midpoint potential ($V_{\mathrm{mid}}$), and total energy (E).

Three correlations in Equations (7)–(9) were developed based on the training set of 22 nitrocompounds. Equation (7) shows the correlation with an R^2 value of 0.83 and an average error of 9%. The predicted impact sensitivity values are compared with experimental data in Table 2:

$$\log(h_{50}) = 7.096(\varepsilon_{\mathrm{LUMO}} - \varepsilon_{\mathrm{HOMO}}) - 7.096\mathrm{MPP} + 0.000529\mathrm{E} + 0.711. \tag{7}$$

The energy difference between LUMO and HOMO is proportional to the impact sensitivity, because a small gap between LUMO and HOMO can facility electron transfer from HOMO to LUMO. The midpoint potential of the longest C–NO_2 bond (V_{mid}) is the electrostatic potential at the midpoint of the C–NO_2 bond. It is invariably positive for nitroaromatics C–NO_2 linkages and is related to the strength

Table 1

Quantum chemical descriptors calculated at HF/STO-3G level

No. (Units)	Material	$\varepsilon_{\mathrm{HOMO}}$ (eV)	$\varepsilon_{\mathrm{LUMO}}$ (eV)	Midpoint potential (eV)	E(total) (Hartrees)	Dipole moment (Debye)	Longest C–NO_2 bond (Angstrom)
1	2,3,4,5,6-pentanitroaniline	–0.31	0.08	0.19	–1285.6	4.27	1.53
2	2,4,6-trinitroresorcinol	–0.28	0.10	0.11	–977.7	2.58	1.50
3	2,3,4,6-tetranitroaniline	–0.30	0.09	0.20	–1085.0	4.28	1.53
4	picric acid	–0.28	0.10	0.13	–903.9	2.61	1.51
5	2,4,6-trinitro-3-aminophenol	–0.28	0.11	0.11	–958.2	1.22	1.49
6	2,2′,4,4′,6,6′-hexanitrobiphenyl	–0.30	0.10	0.16	–1658.9	0.00	1.51
7	2,4,6-trinitrobenzoic acid	–0.30	0.11	0.15	–1015.1	0.67	1.51
8	1,3,5-trinitrobenzene	–0.30	0.12	0.15	–830.0	0.00	1.51
9	picramide	–0.28	0.11	0.12	–884.3	2.00	1.50
10	2,4,6-trinitroanisole	–0.29	0.13	0.13	–942.5	2.65	1.51
11	2,4,6-trinitro-m-cresol	–0.28	0.10	0.13	–942.4	1.50	1.51
12	3,5-dimethyl-2,4,6-trinitrophenol	–0.28	0.11	0.12	–981.0	2.69	1.51
13	1,3-diamino-2,4,6-trinitrobenzene	–0.27	0.13	0.10	–938.7	1.23	1.49

(*Continued*)

Table 1
Continued

No. (Units)	Material	$\varepsilon_{\mathrm{HOMO}}$ (eV)	$\varepsilon_{\mathrm{LUMO}}$ (eV)	Midpoint potential (eV)	E(total) (Hartrees)	Dipole moment (Debye)	Longest C–NO_2 bond (Angstrom)
14	1,3,5 triamino 2,4,6-trinitrobenzene	–0.27	0.15	0.07	–993.0	0.00	1.47
15	2,4,6 trinitrotoluene	–0.30	0.12	0.14	–868.6	1.11	1.51
16	1,1,1,3-tetranitrobutane	–0.30	0.13	0.26	–958.2	4.53	1.56
17	1,1,1,3,5,5,5 heptanitropentane	–0.32	0.12	0.26	–1598.9	4.01	1.56
18	1,1,1,6,6,6-hexanitro-3-hexyne	–0.33	0.13	0.27	–1434.3	2.66	1.56
19	1,1,1,6,6,6-hexanitro-3-hexene	–0.33	0.13	0.26	–1435.5	1.01	1.56
20	3,3,4,4-tetranitrohexane	–0.31	0.14	0.21	–1035.4	0.00	1.57
21	2,2,4,4,6,6-hexanitroheptane	–0.31	0.13	0.22	–1475.4	1.98	1.57
22	2,2,4,6,6-pentanitroheptane	–0.29	0.15	0.21	–1274.7	8.02	1.56

Table 2
Comparison of predicted and experimental impact sensitivity $\log(h_{50})$

Observation	Predicted	Experimental[a]	Residuals	Error (%)
1	1.367	1.176	–0.191	14.0
2	2.096	1.633	–0.462	22.1
3	1.453	1.613	0.160	11.0
4	1.959	1.940	–0.020	1.0
5	2.190	2.140	–0.050	2.3
6	1.538	1.929	0.392	25.5
7	1.973	2.037	0.065	3.3
8	2.106	2.000	–0.106	5.0
9	2.193	2.248	0.055	2.5
10	2.212	2.283	0.072	3.2
11	2.043	2.281	0.238	11.7
12	2.057	1.886	–0.170	8.3
13	2.283	2.505	0.223	9.8
14	2.627	2.505	–0.121	4.6
15	2.199	2.196	–0.003	0.1
16	1.284	1.519	0.234	18.3
17	1.034	0.903	–0.131	12.7
18	1.193	0.845	–0.348	29.2
19	1.243	1.230	–0.013	1.0
20	1.822	1.903	0.081	4.4
21	1.471	1.462	–0.009	0.6
22	1.641	1.748	0.107	6.5

[a] Kamlet and Adolph [5].

of the bond. The more positive the midpoint potential, the more impact sensitive the molecule is. The energy of the molecule also correlates well with the impact sensitivity and indicates the relative stability of the molecule. The lower the energy, the more thermally stable the molecule. However, the correlation shows that molecules with low total energy are more impact sensitive.

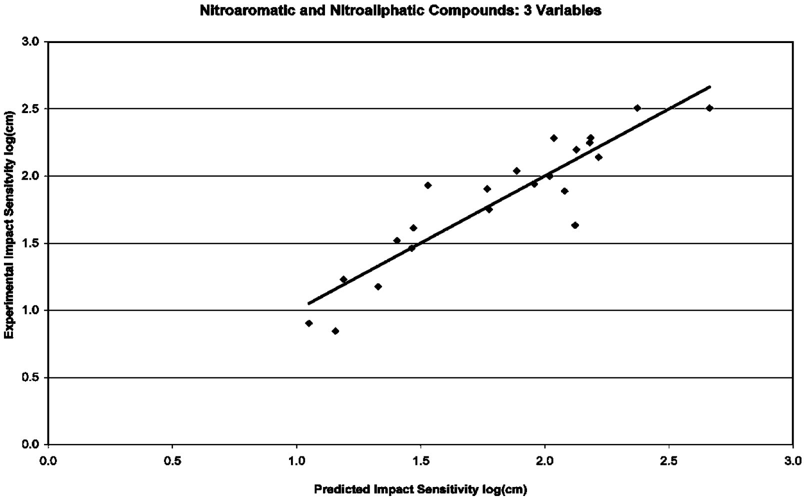

Figure 1. Comparison of predicted with experimental impact sensitivities based on Equation (8).

The second correlation that was developed was based on three molecular descriptors: $\varepsilon_{\mathrm{LUMO}}$, MPP, and E, as shown below:

$$\log(h_{50}) = 7.485\varepsilon_{\mathrm{LUMO}} - 5.922\mathrm{MPP} + 0.000423\mathrm{E} + 2.412. \quad (8)$$

This correlation has an R^2 value of 0.84 with an average error of 9%. Figure 1 displays the predicted sensitivity values against the experimental values. Finally, Equation (9) is based on two molecular descriptors, which are $\varepsilon_{\mathrm{LUMO}}$ and MPP:

$$\log(h_{50}) = 7.941\varepsilon_{\mathrm{LUMO}} - 7.089\mathrm{MPP} + 2.085. \quad (9)$$

This correlation has an R^2 value of 0.81 and an average error of 11%. The experimental and predicted values for this equation are plotted in Figure 2.

These equations show that the three parameters, $\varepsilon_{\mathrm{LUMO}}$, midpoint potential, and total energy of the molecule, are closely related to the impact sensitivities. The $\varepsilon_{\mathrm{LUMO}}$ value, as mentioned above, is the lowest ground state level that does not contain an electron. When $\varepsilon_{\mathrm{LUMO}}$ is relatively low, it is more likely for an electron to move up to that level during a

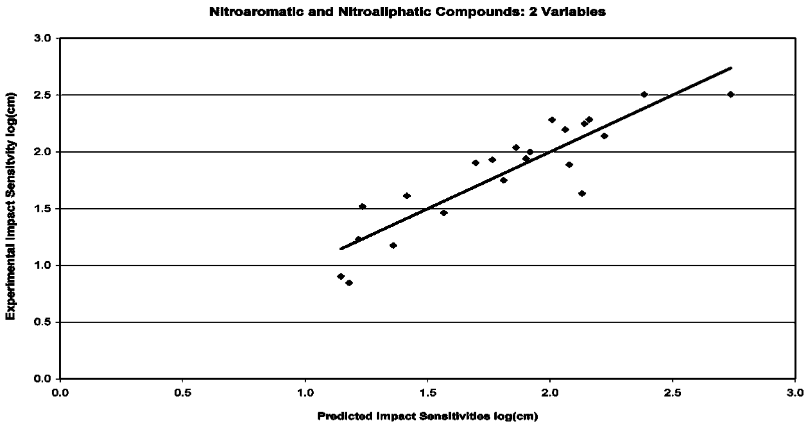

Figure 2. Comparison of predicted with experimental impact sensitivities based on Equation (9).

reaction. The lower the $\varepsilon_{\mathrm{LUMO}}$ value, the more impact sensitive a molecule will be. All three of these parameters are found to correlate well with the impact sensitivity of the molecule.

A correlation using only the seven nitroaliphatic compounds was developed based on the MPP and the E, as shown below:

$$\log(h_{50}) = -9.757\mathrm{MPP} + 0.000922\mathrm{E} + 4.955, \qquad (10)$$

and it has an R^2 value of 0.94 with an average error of 5%. As expected, this equation provides a better correlation because it is based on the same chemical class. Figure 3 displays the predicted values of this equation against the experimental values.

Correlations Using Semiempirical Method

The calculated molecular descriptors using the semiempirical method PM3 are shown in Table 3. The ionization energy is the negative of the energy of HOMO, because it requires energy to remove one electron from HOMO. By comparing Table 3 with Table 1, the values for the same molecular descriptor are different because different levels of theory were used to calculate the properties. Most molecular descriptors are sensitive to quantum chemical models and basis sets, so correlations

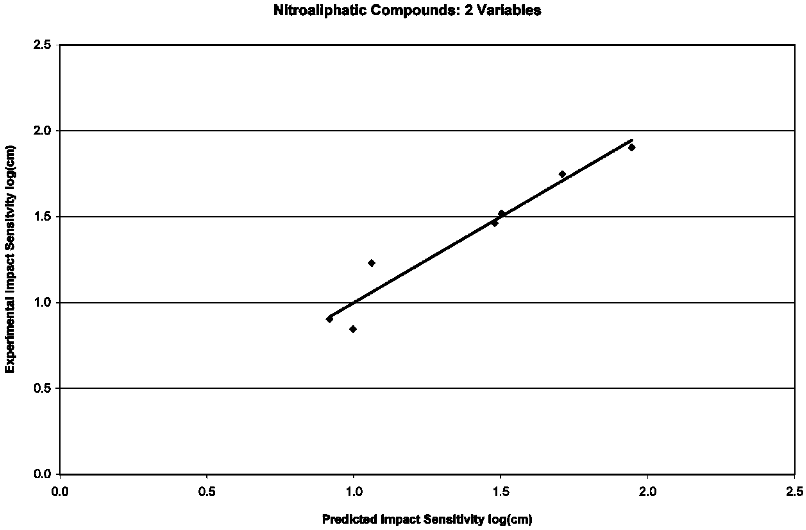

Figure 3. Comparison of predicted with experimental impact sensitivities based on Equation (10) for nitroaliphatic compounds.

must be carried out using the results from the same model and basis set. It is expected that the correlations from different levels of theory and the basis set will differ significantly.

Statistical analysis was conducted on all the descriptors and their combinations. The descriptors that correlate with impact sensitivity are the dipole moment and the ionization energy or the energy of HOMO. Both h_{50} and $\log(h_{50})$ were used as dependent variables, and the corresponding correlations are shown in Equations (11)–(13). Figures 4 and 5 compare predicted values with experimental data based on Equations (12) and (13), respectively. Equation (12) provides a slightly better correlation with R^2 of 0.63 than Equation (13) with R^2 of 0.56:

$$h_{50} = 66.961\varepsilon_{\mathrm{HOMO}} - 21.403\mathrm{DM} + 936.865 \tag{11}$$

or

$$h_{50} = -66.968\mathrm{IP} - 21.403\mathrm{DM} + 936.954, \tag{12}$$

$$\log(h_{50}) = -0.130\mathrm{IP} - 0.296\mathrm{DM} + 5.584. \tag{13}$$

Table 3
Calculated molecular descriptors using the semiempirical method PM3 with MOPAC

No. (Units)	Material	Heat of formation (kJ/mol)	$\varepsilon_{\mathrm{HOMO}}$ (eV)	$\varepsilon_{\mathrm{LUMO}}$ (eV)	E (eV)	Dipole moment (Debye)	Ionization potential (eV)
1	2,3,4,5,6-pentanitroaniline	128.91	–11.01	–3.53	–29875.88	6.67	11.01
2	2,4,6-trinitroresorcinol	–382.77	–11.49	–2.27	–19584.56	1.87	11.49
3	2,3,4,6-tetranitroaniline	52.67	–10.73	–2.92	–23199.29	5.90	10.73
4	picric acid	–172.29	–11.50	–2.51	–17260.97	1.66	11.50
5	2,4,6-trinitro-3-aminophenol	–199.61	–10.37	–1.99	–19467.69	1.86	10.37
6	2,2,4,4,6,6-hexanitrobiphenyl	149.52	–12.31	–2.93	–45706.67	0.08	12.31
7	2,4,6-trinitrobenzoic acid	–295.96	–12.45	–2.82	–20709.01	1.16	12.45
8	1,3,5-trinitrobenzene	28.68	–12.35	–2.53	–15047.18	0.03	12.35
9	2,4,6-trinitroaniline	–1.33	–10.33	–2.21	–17131.67	3.52	10.33
10	2,4,6-trinitroanisole	–95.07	–11.43	–2.34	–19202.47	2.27	11.43

(*Continued*)

Table 3
Continued

No. (Units)	Material	Heat of formation (kJ/mol)	$\varepsilon_{\mathrm{HOMO}}$ (eV)	$\varepsilon_{\mathrm{LUMO}}$ (eV)	E (eV)	Dipole moment (Debye)	Ionization potential (eV)
11	2,4,6-trinitro-m-cresol	–191.98	–11.39	–2.44	–19314.65	0.27	11.39
12	3,5-dimethyl-2,4,6-trinitrophenol	–203.29	–11.21	–2.39	–21482.90	1.33	11.21
13	1,3-diamino-2,4,6-trinitrobenzene	–27.42	–10.03	–1.76	–19308.69	2.90	10.03
14	1,3,5-triamino 2,4,6-trinitrobenzene	–44.96	–10.04	–1.35	–21599.44	0.18	10.04
15	2,4,6-trinitrotoluene	13.11	–11.92	–2.45	–16982.53	1.38	11.92
16	1,1,1,3-tetranitrobutane	–54.70	–12.57	–1.72	–20332.81	3.90	12.57
17	1,1,1,3,5,5,5-heptanitropentane	17.46	–13.11	–1.91	–42991.22	3.73	13.11
18	1,1,1,6,6,6-hexanitro-3-hexyne	198.73	–12.25	–1.63	–34472.57	2.55	12.25
19	1,1,1,6,6,6-hexanitro-3-hexene	51.02	–11.79	–1.56	–35492.82	4.26	11.79
20	3,3,4,4-tetranitrohexane	–17.83	–12.35	–1.42	–25462.51	5.54	12.35
21	2,2,4,4,6,6-hexanitroheptane	–15.63	–12.85	–1.81	–40908.34	1.38	12.85
22	2,2,4,6,6-pentanitroheptane	–80.32	–12.74	–1.20	–33023.64	2.35	12.74

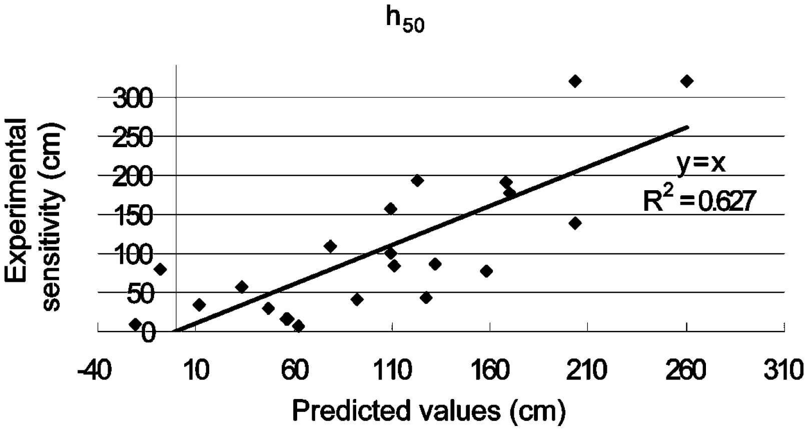

Figure 4. Comparison of predicted with experimental impact sensitivities based on Equation (11).

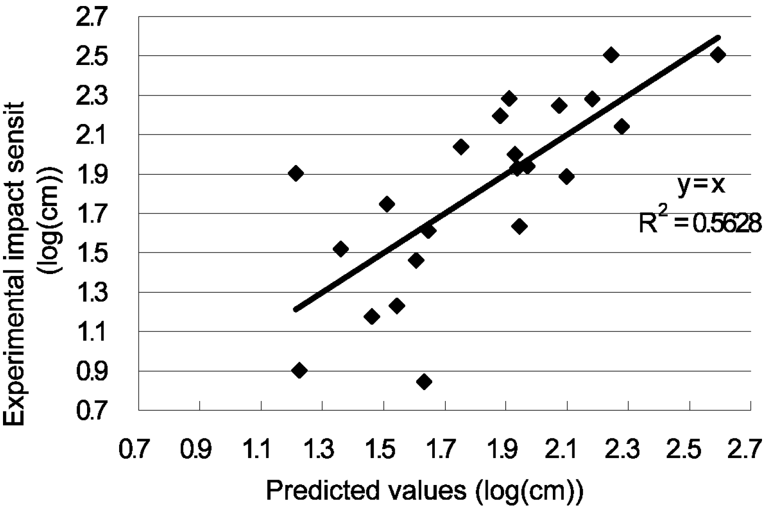

Figure 5. Comparison of predicted with experimental impact sensitivities based on Equation (13).

The impact sensitivity was found to increase with high dipole moment and high ionization potential or the energy of HOMO. The dipole moment is an indicator of the asymmetry of charge distribution within a molecule. If the positive and negative charges in a molecule do not overlap completely and the vector sum of bond polarities is not zero, then the molecule has a dipole moment. The energy of HOMO or ionization potential shows the tendency of a molecule to lose an electron. The correlation shows that the molecule with low HOMO energy is more impact sensitive. The reason behind this relationship is that the C–NO_2 bond is positive and electrophilic and is more easily broken when accepting an electron than losing an electron.

Conclusions

Knowledge about energetic materials has increased dramatically through the years. More importantly, impact sensitivities are becoming more predictable and easier to understand. In this work, correlations with impact sensitivity were developed using quantum chemical molecular descriptors. Both ab initio and semiempirical methods were employed to calculate the molecular properties. The correlations that have been developed here provide a better understanding of impact sensitivity from a molecular level. The correlations can help screen explosives and relate their impact sensitivity with molecular descriptors. Without performing an experiment, the impact sensitivity of a compound can be predicted with a fair accuracy.

Acknowledgments

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