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# Recent Developments for Prediction of Power of Aromatic and Non-Aromatic Energetic Materials along with a Novel Computer Code for Prediction of Their Power

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**Abstract**: The explosive power or strength of an energetic material shows its capacity for doing useful work. This work reviews recent developments for prediction of power of energetic compounds. A new user-friendly computer code is also introduced to predict the relative power of a desired energetic compound as compared to 2,4,6-trinitrotoluene (TNT). It is based on the best available methods, which can be used for different types of energetic compounds including nitroaromatics, nitroaliphatics, nitramines, and nitrate esters. The computed relative powers are consistent with the measured data for some new materials containing complex molecular structures.

**Keywords:** Review · Energetic material · Trauzl lead block test · Ballistic mortar test · Computer code

## 1 Introduction

Detonation parameters containing detonation heat, velocity and temperature as well as the Chapman-Jouguet pressure are usual factors for describing the performance potential of an explosive [1–7]. Different computer codes on the basis of suitable predictive methods have been developed for prediction of detonation performance, sensitivity, and thermochemical properties of different classes of energetic compounds [8–17].

The explosive power of an energetic compound shows its capacity for doing useful work that depends on the expansion of gaseous products for doing work [1, 4]. It can be measured by well-known methods such as ballistic mortar, Trauzl lead block, underwater explosion, cylinder, Hess, Kast and plate dent tests [18–21]. Ballistic mortar and Trauzl lead block tests are simple and convenient methods so that experimental data of many energetic compounds are available. Moreover, several methods have been introduced to predict the power of energetic materials through ballistic mortar and Trauzl lead block tests [22–28]. Among these methods, several predictive methods are suitable for development of a new computer code that they are based on the molecular structure [26], heat of formation [28], the calculated heats of detonation [27], and specific impulse [25].

The purpose of this work is to review some recent developments for prediction of the power of energetic compounds by ballistic mortar and the Trauzl lead block tests. A novel computer code has been introduced to estimate the relative power as compared to 2,4,6-trinitrotoluene (TNT) on the basis of the best available predictive methods for ballistic mortar and the Trauzl lead block tests.

## 2 Different Predictive Methods for Power (Strength) Estimation

The Trauzl lead block test consists of a standard cast cylindrical lead block with 0.200 m height and 0.200 m diameter that can be charged by 10 g of material and a detonator. Details of this test are given elsewhere [29]. The results of this test are not often reproducible and they may show the uncertainties [30].

Heat of explosion and gas volume are two variables that have been used in some predictive methods of the Trauzl lead block test [23, 24, 31]. It was recently indicated that the measured condensed phase heat of formation or the calculated gas phase heat of formation [28], the calculated heats of detonation [27] and specific impulses [25] can be used to estimate volume of expansion in the Trauzl lead block test. Among these methods, the method on the basis of heat of detonation of an energetic compound is more suitable for new computer code. Moreover, the calculation of specific impulse requires another computer code such as ISPBKW [32].

The ballistic mortar is also one of the preferred tests for the explosive power measurements. About 10 g of the explosive charge is initiated in the mortar cavity that is en-

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closed by a steel projectile in which a heavy steel mortar is attached to a pendulum. The mortar is swung from its position after the projectile ejected out of the mortar so that the maximum swing of the mortar can be used to measure the power of a desired explosive.

Oxygen balance and detonation velocity can be related to power as measured by the ballistic mortar [33]. Since the correlation coefficient ($R^2$) of suggested relation is poor, i.e. 0.21, this approach is not reliable. A reliable and simple method has been recently introduced for predicting power by the ballistic mortar test for pure and mixture of energetic materials [26]. This method can be used for different classes of energetic compounds including nitroaromatics, acyclic and cyclic nitramines, nitrate esters, and nitroaliphatics.

## 3 Results and Discussion

### 3.1 The Use of the Calculated Heats of Detonation for Estimation of Power by the Trauzl Lead Block Test

For an explosive having the general formula $C_aH_bN_cO_d$, the simplest way for estimation of the product compositions is based on the "$H_2O$–$CO_2$ arbitrary", which was suggested by Kamlet and Jacobs [34] as:

$$C_aH_bN_cO_d \rightarrow \frac{1}{2}bH_2O + \frac{1}{2}cN_2 + \left(\frac{1}{2}d - \frac{1}{4}b\right)CO_2 + \left(a - \frac{1}{2}d + \frac{1}{4}b\right)C \quad (1)$$

The products of Equation (1) can be used to guess the heat of detonation from the heats of formation of the reactants and detonation products of the detonation through the following relation:

$$Q_{\det,H_2O-CO_2}(kJ/g) = \frac{-\frac{b}{2}\Delta_f H^\theta[H_2O(l)] - \left(\frac{1}{2}d - \frac{1}{4}b\right)\Delta_f H^\theta[CO_2(g)] + \Delta_f H^\theta(\exp losive)}{formula\ weight\ of\ \exp losive} \quad (2)$$

where $Q_{detH_2O\text{-}CO_2}$ is the predicted heat of detonation by the "$H_2O$-$CO_2$ arbitrary", $\Delta_fH^0[H_2O(l)]$ and $\Delta_fH^0[CO_2(g)]$ is the standard heat of formation of $H_2O(l)$ and $CO_2(g)$, respectively, and $\Delta_fH^0$(explosive) is the condensed phase heat of formation of desired explosive. For those energetic compounds where their experimental data of the condensed phase heat of formation are not available, simple empirical [3, 35–39], quantum mechanical [40–43], group additivity [44,45], and artificial neural network [46] methods can be used to find the condensed phase heat of formation of different classes $C_aH_bN_cO_d$ energetic compounds.

For energetic compounds with general formula $C_aH_bN_cO_d$, it was found that the ratios of the number of carbon to oxygen ($r_{a/d}$) and $Q_{detH_2O-CO_2}$ can be used to predict the power in the Trauzl lead block test as follows [27]:

$$\%f_{Trauzl,TNT} = -69.41\, r_{a/d} + 39.69\, Q_{\det,H_2O-CO_2} \quad (3)$$

where $\%f_{Trauzl,TNT}$ represents as the relative strength in the form:

$$\%f_{Trauzl,TNT} = \frac{\Delta V_{Trauzl}(explosive)}{\Delta V_{Trauzl}(TNT)} \times 100$$

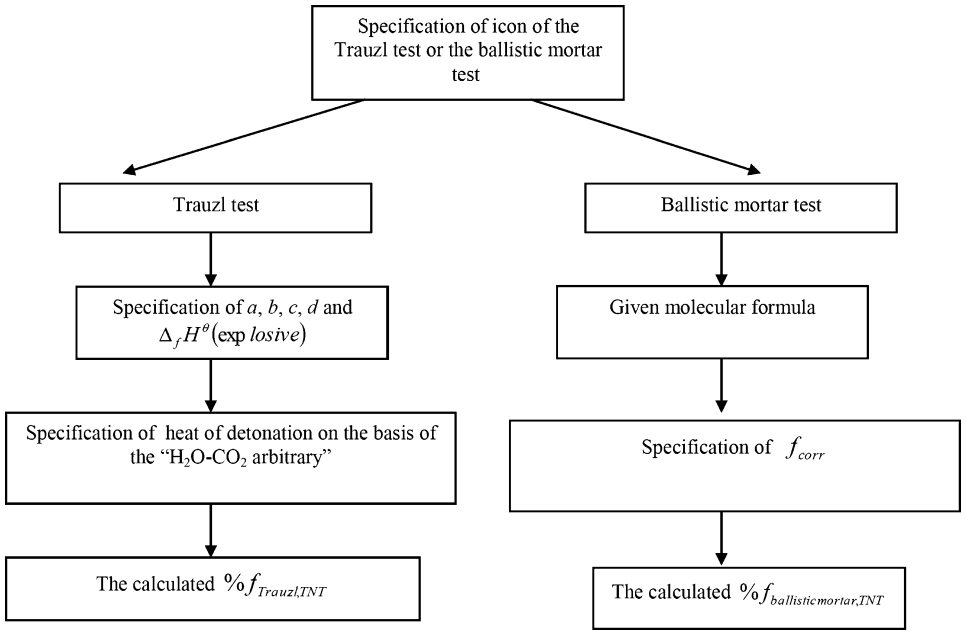



**Figure 1.** Block diagram of the software of the new computer code for calculation of the power of energetic materials.

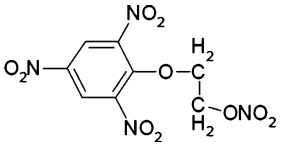
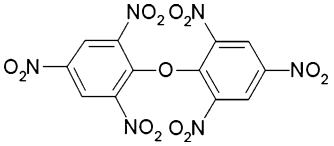
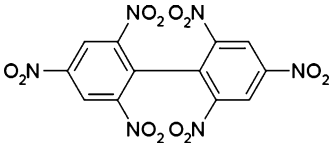
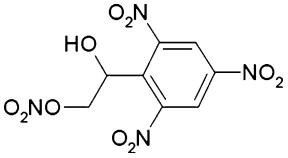
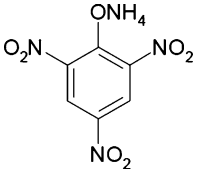
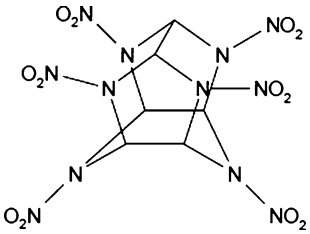
in which $\Delta V_{Trauzl}$(explosive) and $\Delta V_{Trauzl}$(TNT) are the volume of expansion for explosive and 2,4,6-trinitrotoluene (TNT), respectively. The quantity $\%f_{Trauzl,TNT}$ can be used for qualitatively characterizing the strength of an explosive, if the error associated with it remains less than the error associated with $\Delta V_{Trauzl}$. It can be used for quantitative comparison of the effect explosions for different high explosives.

### 3.2 Prediction of Power Using the Ballistic Mortar

For calculation of the power of energetic compounds with the general formula $C_aH_bN_cO_d$ through the ballistic mortar, the following correlation can be used [26]:

$$\%f_{ballisticmortar,TNT} = 113 - 5.16a + 2.79c + 3.61d - 46.18f_{corr} \quad (4)$$

**Table 1.** Comparison of the calculated power as $\%f_{Trauzl,TNT}$ for several complex energetic compounds belong to different classes with the measured values.

| No. | Name | Exp. | $\Delta_fH^0$(explosive) /kJ mol$^{-1}$ | Computer code | Dev. |
|---|---|---|---|---|---|
| 1 | $O_2NOCH_2CH_2OCH_2CH_2OCH_2CH_2ONO_2$ | 108 [29] | −656.9 [52] | 122 | −14 |
| 2 |  | 119 [29] | −277.4 [29] | 123 | −4 |
| 3 |  | 126 [29] | −67.39 [29] | 115 | 11 |
| 4 | Nitrocellulose, 13.3% N<br>Nitrocellulose , 13.3% N | 126 [29] | −1435.1 [29] | 128 | −2 |
| 5 |  | 117 [29] | 68.2 [52] | 114 | 3 |
| 6 |  | 121 [53] | −287.7 [52] | 122 | −1 |
| 7 |  | 95 [29]<br>113 [54] | −371.0 [29] | 95 | 0<br>18 |
| 8 |  | – | 377.4 [55] | 154 | – |

The parameter $f_{corr}$ can be used to correct overestimated values on the basis of elemental composition that can be specified as follows:

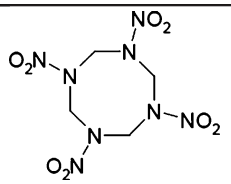
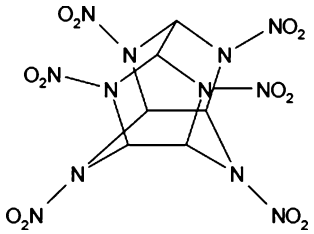
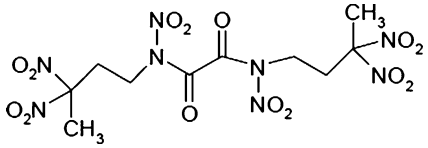
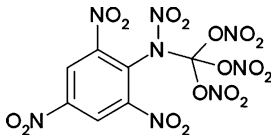
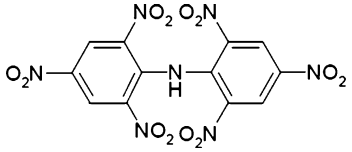
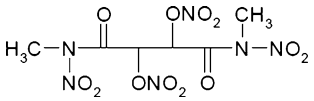
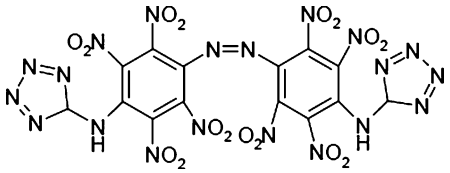
(i) Dinitrosubstituted benzene or those energetic compounds with the condition d $-(a+b/2) \geq 8$: the value of $f_{corr}$ equals 0.7.
(ii) Specific energetic compounds: For those energetic compounds containing one of these situations: (1) a = 0; (2) b = 0, and (3) the presence of the molecular fragment –NH–CO–NH–, the value of $f_{corr}$ is 1.0.

The value of $f_{corr}$ equals zero in Equation (4), if the conditions for giving them the above various values are not met.

### 3.3 Computation of Power of Energetic Materials by New Computer Code

A new computer code was developed to calculate the power of energetic compounds on the basis of two introduced models. It runs on windows operating system using modern modular and object-oriented techniques in Visual Basic 6.0 that occupies about 1.0 MB of hard disk space in the computer. It can be installed under Windows 98, 2000, XP as well as under Windows 7.0 and 8.0. The algorithm of the new computer code is shown in Figure 1 as flow chart for prediction of power of energetic materials. For calculation of $\%f_{Trauzl,TNT}$, the measured condensed phase heat of formation of pure energetic compounds should be given

**Table 2.** Comparison of the calculated power as $\%f_{ballistic\ mortar,TNT}$ for several complex energetic compounds belong to different classes with the experimental data.

| No. | Name | Exp. | Computer code | Dev |
|---|---|---|---|---|
| 1 |  | 150 [56] | 144 | 6 |
| 2 |  | – | 159 | – |
| 3 |  | 129 [57] | 134 | −5 |
| 4 |  | 143 [56] | 145 | −2 |
| 5 | $\{[(O_2NO)CH_2]_3CCH_2\}_2O$ | 144 [56] | 147 | −3 |
| 6 |  | 111 to 115 [56] | 114 | −3 to 1 |
| 7 |  | 131 to 135 [57] | 142 | −11 to −7 |
| 8 |  | – | 154 | – |

as input. The knowledge of the molecular structure of energetic compounds is also the only essential parameter for computation of $\%f_{\text{ballistic mortar,TNT}}$.

### 3.4 Validation of the New Computer Code

#### 3.4.1 The Predicted Values of $\%f_{\text{Trauzl,TNT}}$

The calculated values of $\%f_{\text{Trauzl,TNT}}$ for several energetic compounds containing complex molecular structures are given in Table 1. The validity of the new computer code is good with respect to the measured values. As seen in Table 1, the predicted value of $\%f_{\text{Trauzl,TNT}}$ for hexanitrohexaazaisowurtzitane (CL-20) is equal to 154, which is consistent with its high detonation performance [47,48].

#### 3.4.2 Estimation of $\%f_{\text{ballistic mortar,TNT}}$

The calculated $\%f_{\text{ballistic mortar,TNT}}$ of the new computer code for several complex energetic compounds containing new explosives are given in Table 2. The overall agreement of the new computer code with reported $\%f_{\text{ballistic mortar,TNT}}$ is quite good for a wide range of different classes of energetic. As seen in Table 2, $\%f_{\text{ballistic mortar,TNT}}$ of thermally stable insensitive high explosive *N*,*N*′-bis(1,2,3,4-tetrazole-5-yl)-4,4′-diamino-2,2′,3,3′,5,5′,6,6′-octanitroazobenzene (BTeDAONAB) equals 154, which confirms its high detonation performance as reported elsewhere [49].

#### 3.4.3 Limitations of the New Computer Code

Although the new computer code provides relatively good reliability with respect to the measured data, it has also several restrictions:

(a) It can predict only $\%f_{\text{Trauzl,TNT}}$ and $\%f_{\text{ballistic mortar,TNT}}$ of energetic compounds with general formula $C_aH_bN_cO_d$.
(b) It can be used only for macroscale energetic compounds because nanoscale energetic compounds have different properties with respect to macroscale [50,51].
(c) For those energetic compounds containing unfamiliar molecular moieties, e.g. $-C(NO_2)_3$, the predicted values of $\%f_{\text{Trauzl,TNT}}$ and $\%f_{\text{ballistic mortar,TNT}}$ may be different. In this situation, the estimated power by $\%f_{\text{Trauzl,TNT}}$ is more reliable because it depends only on $r_{a/d}$ and $Q_{\text{detH}_2\text{O-CO}_2}$.

## 4 Conclusions

The new computer code introduces a novel and easy pathway for estimation of the power of an energetic compound by two well-known methods, the Trauzl lead block and the ballistic mortar tests. For many energetic compounds with general formula $C_aH_bN_cO_d$, the predicted results in terms of $\%f_{\text{Trauzl,TNT}}$ and $\%f_{\text{ballistic mortar,TNT}}$ are consistent with each other. For prediction of $\%f_{\text{Trauzl,TNT}}$, the condensed phase heat of formation is an essential input parameter. The predicted results of the new computer can be used to design of energetic coupled with desirable power.

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