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An Algorithm for Evaluation of Potential Hazards in Research and Development of New Energetic Materials in Terms of their Detonation and Ballistic Profiles

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Abstract: In the present paper we report recommendations for safe handling with unknown explosive materials and compositions. These are based on quantum-chemical evaluations of the detonation and ballistic profiles of newly synthesized explosives and their comparison with the known reference compounds. The proposed methodology is rather simple, fast and does not require special skills. Meanwhile, it allows an effective quenching of the potential risk associated with injuries caused by accidental explosions. Additionally, we have developed two utilities, which significantly simplify the calculation process. The proposed algorithm was found to be more successful in estimation of detonation velocity of several common explosives in comparison with commercially available software EMDB, EXPLO5 and Cheetah 8.0. The reported results will be useful for scientific personnel working in the field of development and testing of explosives.

Keywords: chemical safety · energetic materials · detonation and ballistic properties · theoretical analysis

1 Introduction

Current industrial, military and scientific applications require effective high-energy density materials (HEDM), which satisfy the tight criteria of environmental safety and possess high detonation performance [1–3]. Research and development of a new HEDM undergoes scientists of a potential risk of injuries; therefore, a comprehensive safety program for research laboratories was recently proposed [4]. These risks can be associated with the both accidental explosions and unsatisfied protective measures. Often these two factors appear simultaneously. Such accidents happen with frightening regularity leading to serious disorders and often leaving workers permanently disabled. For example, an attempt to clean mechanically the valve contaminated with dried aryl diazonium salts resulted in injury of two workmen [5]. The reason of this accident was in a lack of knowledge about impact sensitivity of crystalline diazoniums salts and the study of this phenomenon was performed only after the accident. By the way, the computer prediction of impact sensitivity becomes today a "double-click" procedure, since a number of theoretical models are already developed and tested [6].

Work with small quantities of explosives, however, does not guarantee that serious injuries cannot be obtained. Thus, a student-chemist lost both hands and one eye when manipulating with explosives in the laboratory [7]. Unfortunately, similar accidents are regularly described in the literature [8,9]. In contrast to bomb suits, which are necessary for military and some civilian applications assuming large-scale explosive charges (0.227–0.567 kg) being applied [10], in the laboratory, the most frequently injured parts of human body are hands and eyes. Therefore, safety gloves and ballistic eyewear are the most important personal protective equipment (PPE). In the case of chemical and biological hazards, comprehensive decision logic for selection of protective clothing was developed earlier [11]. Conversely, the choice of PPE for explosive applications still remains to be a serious challenge for scientists.

Thus, Klapötke et al. [12,13] tested safety gloves using explosions of 1 g of lead azide in a 10 mL flask. He found that double-glove combination provides sufficient protection, but a wider test series must be carried out to elaborate standardized testing protocol [13]. Murray et al. [14,15] also performed such tests for hand, eye, face and body protection and found that in the relative vicinity between the operator and explosive material, even small quantities of the latter (0.3 g) can lead to serious injuries. For ballistic eyewear, however, these norms already exist and according

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them, the eyewear must be resistant to a 0.15 caliber T37 shaped projectile at a velocity of 640–660 ft/s [16].

Level of protection provided by PPE is usually established on the basis of existing standards of explosives (Figure S1 in ESI). Detonation properties of RDX and HMX (chemical names are given in Table S1 in ESI) are generally applied as reference values for comparison with the predicted or newly synthesized explosives, which often are much more powerful. Recently, we have predicted single-bonded crystalline phase of nitrogen, which demonstrate the calculated detonation pressure and velocity equal to 146.06 GPa and 15.86 km/s, respectively [17]. Similar values demonstrate the other allotropes of nitrogen including molecular crystals [18]. When handling such powerful explosives, the safety criteria become tighter and the only way to estimate an appropriate level of protection is to perform quantum-chemical calculations.

In the present paper we have focused on the safety norms and regulation which directly depend on the detonation properties of explosive materials. The purpose of this article is to describe a clear methodology allowing experimentalists to perform quantum chemical calculations from scratch.

2 Affected Norms and Regulations

Apart of the norms for PPE described in the previous section, there are several linear parameters, which determine personnel safety during surface mining blasting applications. These parameters directly related with the detonation properties of the explosives applied. Thus, the distance r_{scatt} (m), which is dangerous for people due to scattered of individual pieces of rock, can be expressed as the following [19]:

$$r_{scatt} = 1250\eta_{expl}\sqrt{\frac{f}{1+\eta_{fill}}\frac{d}{a}} \quad (1)$$

where, η_{expl} and η_{fill} are the coefficients of a blast-hole filling with explosive and filler, respectively; f is the coefficient of rock strength according to the Protodyakonov scale; d is the hole diameter; a is the distance between the holes in a row or between the rows (m).

The coefficients η_{expl} and η_{fill} can be expressed as in eq 2 and 3:

$$\eta_{expl} = l_{expl}/L, \quad (2)$$

$$\eta_{fill} = l_{fill}/L_{stemm}, \quad (3)$$

where, l_{expl} and l_{fill} are the heights of explosive and filler; L and L_{stemm} are the hole depth and stemming height, respectively [19].

Another important parameter is the distance r_D (m), which excludes the possibility of detonation transferring from the explosion on the ground surface. It is determined by the formula [19].

$$r_D = K_D\sqrt[3]{Q}\sqrt[4]{b} \quad (4)$$

Herein, K_D is the coefficient, which depends on the nature of explosive; Q is the mass of the active explosive (kg); b is the less linear size of the passive charge (stack width).

Finally, the chemical hazard of the explosive gases can be quantified *via* the safe distance r_{gas} (m), which excludes the action of toxic gases after explosion; this can be expressed by the formula [19]:

$$r_{gas} = 160 \cdot \sqrt[3]{Q} \cdot (1 + 0.5v_w) \quad (5)$$

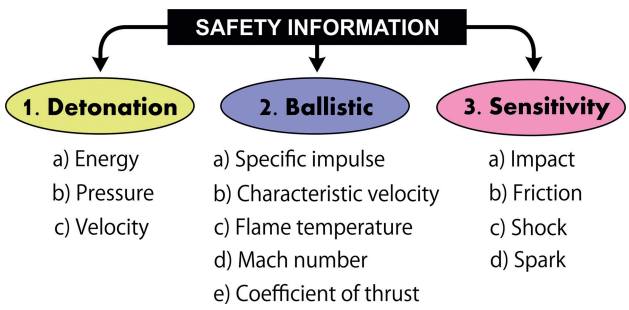
where v_w is the wind speed. In perpendicular direction to the wind and during calm the term $(1+0.5v_w)$ equals to unity.

Moreover, in the Ukrainian regulations on civil blasting, there are other prescribed norms which are directly related with the detonation power of explosives [20]. Thus, safe work with unknown energetic materials assumes estimation and comparison of three main groups of properties, which are presented in Scheme 1. The aim of the present paper is to provide recommendations for estimation algorithm which covers the first two groups of properties before these will be examined experimentally according to the developed protocols [21]. The sensitivity parameters, however, also form a very important group of factors, which can be the reason of accidental explosions, but this requires a more specialized consideration and cannot be described in terms of the present paper.

3 Results and Discussion

3.1 Detonation Profile

The main detonation properties of an explosive include detonation velocity (D, m/s) and pressure (P, GPa). There are



Scheme 1. The main elements of the safety information of explosives.

many approaches in the literature which allow calculating these quantities. In this paper we do not intend to provide a fully comprehensive review but we should highlight contribution of Keshavarz who published about 40 individual papers on different quantitative "structure-property" relationships (QSPR) in the field of detonation performance and sensitivity of explosives. These methods are well reviewed in two recent books [22,23]. Moreover, on the basis of these QSPRs, a program package EMDB was recently developed providing more than 30 properties of HEDM [24]. This program has a serious advantage in comparison with other popular commercially available software, EXPLO5 [25] or Cheetah 8.0 [26], since it does not need any input information other than a molecular structure. Therefore, in the present work, we describe an algorithm which does not require any numerical input data as well. The key point in this algorithm is the empirical scheme developed by Kamlet and Jacobs (eqs 6 and 7) [27]:

$$D = 1.01\left(N\bar{M}^{1/2}Q^{1/2}\right)^{1/2}(1 + 1.30\rho_0) \quad (6)$$

$$P = 1.558\rho_0^2 N\bar{M}^{1/2}Q^{1/2}, \quad (7)$$

where N and $\overline{M}$ are the dimensionless structure-derived quantities. These parameters, together with the detonation energy (Q, cal/g) value, can be calculated in three ways depending on an appropriate structural criterion, which depends on the empirical formula. For the general case of $C_aH_bO_cN_d$ composition these variations of the N, $\overline{M}$ and Q parameters are the following [27]:

Criterion I: $c \geq 2a + b/2$:

$$N = (b + 2c + 2d)/4MW \quad (8a)$$

$$\bar{M} = 4MW/(b + 2c + 2d) \quad (9a)$$

$$Q = (28.9b + 94.05a + 239\Delta H_f^0)/MW \quad (10a)$$

Criterion II: $2a + b/2 > c \geq b/2$:

In this case, the parameter N is described as in eq 8a.

$$\bar{M} = (56d + 88c - 8b)/(b + 2c + 2d) \quad (9b)$$

$$Q = (28.9b + 94.05(c/2 - b/4) + 239\Delta H_f^0)/MW \quad (10b)$$

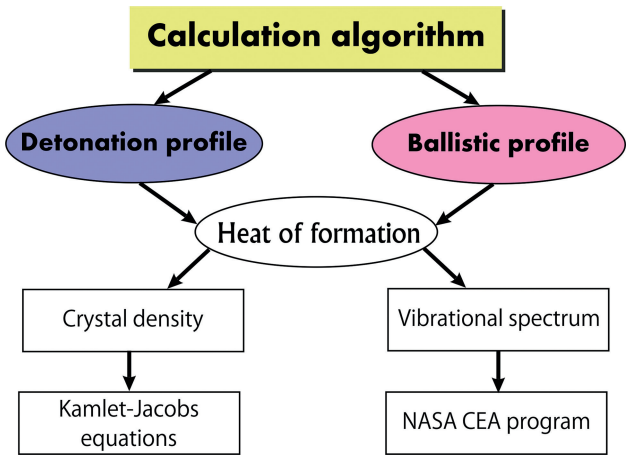
Criterion III: $b/2 > c$:

$$N = (b + d)/2MW \quad (8c)$$

$$\bar{M} = (2b + 28d + 32c)/(b + d) \quad (9c)$$

$$Q = (57.8c + 239\Delta H_f^0)/MW \quad (10c)$$

Herein, MW stands for molecular weight and ΔH_f^0 is the standard solid-state enthalpy of formation. Thus, the latter quantity along with the crystal density ρ (g/cm^3) becomes the only value which must be calculated (see Scheme 2).



Scheme 2. Principal stages of the theoretical analysis of an explosive.

Let us first consider the crystal density. Actually, this problem can be reduced to the condensed (not necessarily solid) phase density since the difference between the solid and liquid phase densities are usually small. In this case, one can simply estimate the volume of a molecule as an isosurface of a defined value of the electron density (usually 0.001 a.u.) which can be carried out using freely distributed Multiwfn program code [28]. Of course, one can apply more sophisticated methods which include the Monte Carlo simulation of a mole of the condensed molecules or to perform a crystal structure prediction for a set of the most frequently appeared space groups (usually $P\bar{1}$ and $P2_1/c$ which cover more than a half of entries in the Cambridge Structural Database) [29]. But these methods require more specialized skills and are time-consuming. Note that the calculations should be performed for the predicted molecule and for a reference molecule to estimate absolute error of the calculation. If this correction is done, even the simplest approach based on the molecular volume estimation can produce reliable results. Thus, all you need is a file with extension *.wfn, which can be generated automatically when using PC GAMESS or Firefly [30] codes for *ab initio* or DFT calculations. The Gaussian users can format the corresponding *.chk file using FormChk utility and obtain an *.fch file which can be used as an input for Multiwfn program. Herein, we do not present detailed tutorials for using the above-mentioned software since it can be found elsewhere.

Similarly, the value of standard enthalpy of formation ΔH_f^0 can also be calculated in a few ways. The simplest way is to obtain a semi-empirically derived value of the gas-phase enthalpy of formation at 0 K. This option is available for different semi-empirical codes (MOPAC, HyperChem,

etc.). The value obtained this way, however, can be reliable only for the known families of compounds for which the methods are parameterized. For unknown classes of compounds, especially when new types of chemical bonds are present, the semi-empirical methods can suffer from a lack of appropriate parameterization; therefore, one should apply *ab initio* or DFT methods. One of the most popular approaches is the complete basis set (CBS) method which is realized in GAUSSIAN program suite [31]. This allows obtaining gas-phase ΔH_f^0 values at 298 K.

Finally, it is necessary to calculate the solid-state enthalpy of formation since real explosive samples are usually crystalline materials. In general case, this transformation is done as in eq 11.

$$\Delta_f H^\circ_{\text{solid}} = \Delta_f H^\circ_{\text{gas}} - \Delta H_{\text{sub}}, \quad (11)$$

Where ΔH_{sub} stands for the sublimation energy. Again, there are several approaches to obtain the latter quantity. The most popular include estimation of the sublimation energy *via* molecular electrostatic potential (eq 12) [32]:

$$\Delta H_{\text{sub}} = \alpha A^2 + \beta\sqrt{v\sigma^2_{\text{tot}}} + \gamma, \quad (12)$$

where A is the molecular surface as described above; σ_{tot} is total molecular electrostatic potential; ν is the charge balance; α, β and γ are the least-squares fit coefficients. The sublimation energy values can be calculated using the Multiwfn program. It is worth noting that in the case of liquid explosive material the sublimation energy must be replaced by the corresponding vaporization energy (ΔH_{vap}) [32]:

$$\Delta H_{\text{vap}} = \alpha\sqrt{A} + \beta\sqrt{v\sigma^2_{\text{tot}}} + \gamma. \quad (13)$$

Another approximation for obtaining the ΔH_{sub} values is based on first-principles calculations of the corresponding crystal structure [33]. Thus, in this case one should have a predicted crystal structure of the studied explosive. Within this approach the ΔH_{sub} values are expressed *via* the lattice energy E_{latt} as in eq 14.

$$\Delta H_{sub}(T) = -E_{latt} - 2RT \quad (14)$$

Herein, the E_{latt} can be calculated as the following:

$$E_{latt} = \frac{E_{solid}}{Z} - E_{gas}, \quad (15)$$

where E_{solid} is the total energy of an asymmetric cell, Z is the number of formula units per asymmetric cell, and E_{gas} is the total energy of a formula unit in the gas phase.

Once the calculation of crystal density and solid-state enthalpy of formation is done, one can easily calculate detonation energy, pressure and velocity using equations which are presented above. Since these computations are time-consuming we have developed a PascalABC.NET routine (for C–H–N–O explosives), which analyzes the corresponding structural criterion for a given chemical formula and prints all the data, namely, N, $\overline{M}$, Q, D and P values. The input file (*input.txt*) for RDX looks like this:

```
3       {C}
6       {H}
6       {N}
6       {O}
79.1    {heat of formation, kJ/mol}
1.82    {crystal density, g/cm3}
```

The corresponding output file (*output.txt*) also contains the value of oxygen balance and other information.

```
EMPIRICAL FORMULA EXPRESSION   :  C H N O
                                   a b c d

_____________________________________________________

EXPLOSIVE FORMULA              :  C3H6N6O6
MOLECULAR WEIGHT               :  222.11748 g/mol
EXPLOSIVE STRUCTURAL CONDITION :  2a + b/2 > d >= b/2
INTERNAL OXIDATION ABILITY     :  Moderate
OXYGEN BALANCE                 :  -21.610185744949 %
_____________________________________________________

CRYSTAL DENSITY                :  1.82 g/cm3
ENTHALPY OF FORMATION (298 K)  :  79.1 kJ/mol

_____________________________________________________

N                              :  0.0337659152264829
M                              :  27.2
DETONATION ENERGY (Q)          :  1500.91699221 cal/g
DETONATION PRESSURE (P)        :  35.208826005021 GPa
DETONATION VELOCITY (D)        :  8.879860494354 km/s
```

Despite the apparent complexity of the discussed calculations, the appropriate skills of a researcher and powerful hardware allow reducing the time for preliminary theoretical study to several hours. On the other hand, the effect of these analyses is very important in terms of occupational safety criteria. A brief analysis of the literature data for the last few years provides a solid understanding that the era of RDX and HMX gradually ends. Today, the more and more novel explosives with enhanced detonation properties, which exceed those of RDX and HMX are synthesized (Table S2 in ESI). Thus, the potential risk of injuries substantially rises and the safety criteria must become tighter.

Summarizing this section, we present results on prediction of the D (m/s) values for several common explosives in comparison with ones recently obtained using EMDB software (Table 1). The calculation details and statistical treatment of the results along with ones previously obtained with EXPLO5 and Cheetah 8.0 software are presented in Tables S3–S6, Figure S2 and Scheme S1 in ESI. We should stress that our method exhibit better results compared to the EMDB software. The EXPLO5 code gives statistical estimates being similar to ones obtained for our method, but this software does not predict crystal density and solid-state enthalpy of formation; therefore, such comparison is not reasonable. Finally, the above-mentioned calculations were performed on a personal computer and took

Table 1. The calculated values of *D* (m/s) for several common explosives obtained using the EMDB v1.0 software [24] and according to our algorithm.

Explosive	Experiment [24]	EMDB v1.0 [24]	Present work
TNT	7026	7230 (3%)	7101 (1%)
HNS	7200	7620 (6%)	7482 (4%)
RDX	8833	8670 (−2%)	8943 (1%)
ε-CL-20	9570	9600 (0%)	9668 (1%)
TKX-50	9432	9140 (−3%)	9890 (5%)
NTO	8335	8080 (−3%)	8167 (−2%)
DAAF	8110	7960 (−2%)	7913 (−2%)

about 7 hours, amounting to approximately one hour for one explosive on average.

3.2 Ballistic Profile

Typical ballistic properties of a material include those listed in Scheme 1. As it follows from Scheme 2, the algorithm for ballistic properties calculation assumes obtaining of the molecular vibrational spectrum. Similarly to the previous section, the vibrational spectrum is necessary for obtaining thermodynamic functions, but in this case one should extract a temperature dependence of three thermodynamic functions, namely, isobaric heat capacity (C_p), enthalpy (H) and entropy (S). These data should be first collected in the tabulated form and then converted to so-called NASA 9 coefficients as the least square fit coefficients ($a_1 \ldots a_9$) for the polynomials of the following forms (eqs 16–18) [34]:

$$\frac{C_p^\circ}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \qquad (16)$$

$$\frac{H^\circ}{RT} = -a_1 T^{-2} + a_2 T^{-1} + \ln T + a_3 + a_4 \frac{T}{2} + a_5 \frac{T^2}{3} + a_6 \frac{T^3}{4} + a_7 \frac{T^4}{5} + \frac{a_8}{T} \qquad (17)$$

$$\frac{S^\circ}{R} = -a_1 \frac{T^{-2}}{2} - a_2 T^{-1} + a_3 lnT + a_4 T + a_5 \frac{T^2}{2} + a_6 \frac{T^3}{3} + a_7 \frac{T^4}{4} + a_9 \qquad (18)$$

The tabulated data on the functions $C_p(T)$, $H(T)$ and $S(T)$ along with the $\Delta_f H^0_{solid}$ value should be presented in a file with extension *.i97. Herein, we do not discuss the structure of this file since it can be found elsewhere. Of course, one can manually calculate the $C_p(T)$, $H(T)$ and $S(T)$ at different temperatures using the known equations (see handbooks on physics of molecules), but this procedure is very painstaking and it takes much time. Therefore, specialized software was developed to transform the information from vibrational spectrum to an *.i97 file. One of the most convenient codes is GPOP (Gaussian Post Processor) [35]. It converts *.out or *.log files (GAUSSIAN output files) to the corresponding *.i97 file. Again, a detailed description of the program can be found at the software website.

Once an *.i97 file is created, it then should be converted to the corresponding *.c97 file in which the NASA 9 coefficients are presented in a specialized form. This can be done using PAC99 code, which may be found in both the GPOP list of routines and the NASA CEA (Chemical Equilibrium with Applications) program package [36]. When the NASA 9 coefficients are obtained for a given compound, these should be transferred to a *thermo.inp* file. This file contains thermodynamic data (in the text form) on all the chemical species, which can be handled by the CEA program. But to complete defining of a new reactant, the *thermo.inp* file should be reformatted into the corresponding *thermo.lib* file, which can be used directly for the calculations with the CEA program. This can be done by a simple run of the CEA program (see the program manual for details). At this stage, everything is ready for calculation of the ballistic properties based on the spectral data obtained by means of the of an isolated molecule calculation.

To obtain more correct spectral characterization of a material, one should calculate vibrational spectrum for its crystalline state. In the case of polymorphism of explosives this is the only way to distinguish their physical properties [6]. In this context, we have developed a PascalABC.NET routine for transformation of the spectral data derived form two very popular programs for periodic calculations, namely, CASTEP and DMol^3 as implemented in Materials Studio 7.0 program suite [37]. The spectral data obtained by these programs should be exported in the form of comma-separated (*.csv) files and then the data should be copied and pasted into an *input.txt* file of the following form:

```
1            {1 - CASTEP, 2 - DMol3}
0.524032227  {ZPVE (eV) - CASTEP, (kcal/mol) - DMol3}
4            {units per asymmetric cell}
79.1         {heat of formation (kJ/mol)}
3            {C}
6            {H}
6            {N}
6            {O}

Spectral data within the temperature range 100-6000 K
```

In this example we demonstrate an input file to convert data obtained from a CASTEP calculation of an RDX crystal. As a result, the program creates an *.i97 file and also a *.thermo file with tabulated data at 298 K. This is very useful since the CASTEP output does not contain explicit thermodynamic data at standard temperature. Finally, the obtained *.i97 file then should be transformed in the same way as described above. Now, having a *thermo.lib* file with the defined new reactant, one can create an input file for the CEA program. This file has extension *.inp while the corresponding output file has extension *.out. Description of these files can be found in the program manual [38]. Thus, a number of very important ballistic properties can be easily calculated, which allows estimation of the potential hazards for an explosive under development.

4 Conclusions

Summing up, we presented in this paper a schematic algorithm for calculation of the detonation and ballistic profiles of explosives or any other materials. Of course, we do not state that this approach is the only correct. The proposed algorithm includes a part of quantum-chemical calculations (structure optimization and vibrational spectra predictions) and post-SCF computations. Due to a rising interest to energetic materials in extreme conditions including nitrogen allotropes [17, 39] or polyguanidine-based monolayers [40], the safety problem becomes a crucial point in the experimental study. In order to facilitate the process of ballistic properties estimation for such periodic materials, we have developed a utility, which can be obtained from the corresponding author.

Despite the discussed detonation and ballistic properties, which determine the power of energetic materials, there is another very important safety criterion, namely, sensitivity. Obviously, this problem is multifaceted and challenging and it deserves a separate discussion. On one hand, the theoretical analysis of sensitivity phenomenon requires some specialized skills. Moreover, the choice of empirical sensitivity model may become critical due to their variety. On the other hand, sensitivity parameters are even more important than the detonation and ballistic properties in terms of occupational safety. Thus, the development of a simple and versatile algorithm for theoretical estimation of sensitivity (mainly impact sensitivity), which can be applicable for both the molecular and solid-state approaches, is of great importance and becomes the issue of further study.

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