A new computer code to evaluate detonation performance of high explosives and their thermochemical properties, part I

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ABSTRACT

In this paper a new simple user-friendly computer code, in Visual Basic, has been introduced to evaluate detonation performance of high explosives and their thermochemical properties. The code is based on recently developed methods to obtain thermochemical and performance parameters of energetic materials, which can complement the computer outputs of the other thermodynamic chemical equilibrium codes. It can predict various important properties of high explosive including velocity of detonation, detonation pressure, heat of detonation, detonation temperature, Gurney velocity, adiabatic exponent and specific impulse of high explosives. It can also predict detonation performance of aluminized explosives that can have non-ideal behaviors. This code has been validated with well-known and standard explosives and compared the predicted results, where the predictions of desired properties were possible, with outputs of some computer codes. A large amount of data for detonation performance on different classes of explosives from $C-NO_2$, $O-NO_2$ and $N-NO_2$ energetic groups have also been generated and compared with well-known complex code BKW.

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1. Introduction

Predicting performance and thermochemical properties of a new energetic compound and its mixture with the other energetic components are very important for the scientists working in the field of high energy materials. Computer codes are recognized to be cost-effective, environmentally desirable and time-saving in the decision to whether it is worth the effort to attempt a new or complex synthesis. Prediction of the performance and thermochemical aspects of new energetic materials from a given molecular structure without using experimental measurement should be evaluated prior to their actual synthesis because it reduces the costs associated with synthesis, test and evaluation as well as hazards of energetic materials.

Various thermodynamic and detonation parameters can be predicted by thermochemical/hydrodynamic computer codes such as BKW [1], RUBY [2] and latter's offspring TIGER [3], CHEQ [4], and CHEETAH [5] (a C version of TIGER), which use empirical equations of state such as Becker–Kistiakosky–Wilson (BKW-EOS) [6], Jacobs–Cowperthwaite–Zwisler (JCZ-EOS) [7] or Kihara–Hikita–Tanaka (KHT-EOS) [8]. The BKW-EOS in spite of

its weak theoretical basis is used extensively. The BKWC-EOS [5], BKWS-EOS [9] and BKWR-EOS [10] are three different parameterizations of the BKW-EOS. The LOTUSES is also a simple computer code, on the basis of empirical models, which has been developed for the prediction of gas phase heat of formation, heat of explosion, volume of explosion gaseous products and other related performance parameters [11–14].

The purpose of this work is to introduce a new computer code on the basis of recent developments of the predictive methods of performance and thermochemical properties of energetic materials, which can complement the computer outputs of the other codes. This computer code can be named evaluation detonation performance of high explosives and their thermochemical properties (EDPHT). In contrast to the other complex thermochemical/hydrodynamic computer codes such as CHEETAH [5], CHEQ [4], TIGER [3], etc., EDPHT is based on the recent simple and reliable empirical methods, which can complement the computer outputs of the other thermodynamic chemical equilibrium codes. It uses the suitable models for prediction of performance of energetic compounds if their measured heat of formation were not available. The EDPHT can use new methods to predict velocity of detonation, detonation pressure, heat of detonation, detonation temperature, Gurney velocity, adiabatic exponent and specific impulse of high explosives. The most important aspect of the present work is that this computer code can be used to predict detonation performance of aluminized explosives, which has

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significantly different detonation properties than those predicted by thermochemical/hydrodynamic complicated computer codes without considering partial equilibrium. For those properties that can be calculated by the other well-kwon codes, this code has been validated with well-known and standard explosives and compared the predicted results with experimental data. Detonation velocity and pressure for different classes of explosives, where experimental data were available, with different C–NO$_2$, O–NO$_2$ and N–NO$_2$ energetic groups have also been compared with well-known complex code BKW.

2. Theory

Performance and thermochemical properties can be specified through different approaches. Recent reliable methods for prediction of these parameters were used in EDPHT computer code. The EDPHT can predict heat of detonation, detonation pressure and velocity, detonation temperature, adiabatic exponent, specific impulse as well as detonation velocity and pressure in aluminized explosives. These properties and corresponding different simple models, which have been used in EDPHT, can be reviewed shortly.

2.1. Heat of detonation

Decomposition of an energetic material will raise the temperature of gaseous products, which will in turn cause them to expand and work on surroundings. The effectiveness of an explosive depends on the amount of energy available in it and the rate of its release. Heat of detonation can be determined from the heats of formation of the reactants and the products of detonation through the relation:

$$Q_{det} \cong \frac{-[\Delta H_f(\text{detonation products}) - \Delta H_f(\text{explosive})]}{\text{formula weight of explosive}} \quad (1)$$

The heat of detonation requires the heat of formation of the explosive which can be estimated from the experimentally derived group additivity quantities [15]. To calculate heat of detonation from Eq. (1), the assumed or computed equilibrium composition of gaseous products would be needed. To predict the problem of decomposition products, LOTUSES [11] computer code uses a set of rules was developed by Kistiakowsky and Wilson [16]. If the condensed phase heats of formation of energetic compounds were reported or estimated [17–19], Eq. (1) with appropriate decomposition paths [20] can be used to calculate heat of detonation.

The heat of detonation can be calculated without using any experimental and computed data of explosive. For non-aromatic and aromatic C$_a$H$_b$N$_c$O$_d$ explosives, with the H$_2$O in liquid state, the following correlations can be used, respectively [21]:

$$Q_{det}(\text{kJ g}^{-1}) = \frac{58.72a - 55.01b - 21.23c + 250.9d + 4.485\,\Delta H_f(g)}{\text{MW}}$$
$$(2)$$

$$Q_{det}(\text{kJ g}^{-1}) = \frac{61.78a - 51.32b - 30.66c + 90.45d - 0.279\,\Delta H_f(g)}{\text{MW}}$$
$$(3)$$

where MW is the molecular weight and ΔH_f (g) is the gas phase heat of formation of energetic compound which can be calculated of explosive by Joback's group additivity method [22,23]. However, the calculated heat of detonation by this method is better than those obtained by Kamlet and Jacobs procedure [24].

2.2. Detonation pressure and velocity

Heat of detonation through Eq. (1) on the basis of suitable decomposition products [20] can be used to predict detonation pressure and velocity [20,25]:

$$P = 15.88\alpha(MQ_{det})^{1/2}\rho_0^2 - 11.2 \quad (4)$$

$$D = 1.404\alpha^{1/2}(MQ_{det})^{1/4}\rho_0 - 1.97 \quad (5)$$

where P is the C-J detonation pressure in kbar, D is detonation velocity in km/s, α is the number of moles of gaseous products of detonation per gram of explosive, M is the average molecular weight of gaseous products and ρ_0 is loading density. It was indicated [20,25] that Eqs. (4) and (5) can predict more reliable results at loading density less than 1.0 g/cm^3 than those of Kamlet and Jacobs [14].

Two simple empirical relationships [26,27] have been recently introduced between detonation pressure and velocity at any loading density and chemical composition of a high explosive as well as its gas phase heat of formation, which can be calculated by Joback's group additivity rule [22,23]. These correlations may be applied to any explosive that contains the elements of carbon, hydrogen, nitrogen and oxygen without using any assumed detonation products and experimental data. The predicted detonation pressure and velocity for both pure and explosive formulations show good agreement with respect to measured values over a wide range of loading densities. Detonation pressure and velocity have the following forms, respectively [26,27]:

$$P = -2.6 + \left(\frac{-1026a + 226b + 1031c + 3150d + 30.7\,\Delta H_f(g)}{\text{MW}}\right)\rho_0^2$$
$$(6)$$

$$D = 1.9 + \left(\frac{-2.97a + 9.32b + 27.68c + 98.9d + 1.22\,\Delta H_f(g)}{\text{MW}}\right)\rho_0$$
$$(7)$$

where P and D are in kbar and km/s, respectively.

2.3. Detonation temperature

To calculate the detonation temperature, it would be needed to use the heat of formation of the explosive [16]. If the condensed phase heats of formation of explosives are known, suitable pathways can be selected for prediction of detonation temperature. To predict detonation temperatures of C$_a$H$_b$N$_c$O$_d$ explosives, the following equations corresponding to four decomposition paths [20] can be used [28]:

$$T_{det} = 298 + \frac{\Delta H_f(c) - 529.4d}{10.95 \times 10^{-3}a - 0.1132b + 13.35 \times 10^{-3}c - 99.1 \times 10^{-3}d}$$
$$(8a)$$

$$T_{det} = 298 + \frac{\Delta H_f(c) - 943.4a + 1229.5d}{-0.1914a + 59.67 \times 10^{-3}b + 16.87 \times 10^{-3}c + 0.2224d}$$
$$(8b)$$

$$T_{det} = 298 + \frac{\Delta H_f(c) - 1158.3a - 252.3b + 847.9d}{-0.2964a - 55.09 \times 10^{-3}b + 18.66 \times 10^{-3}c + 0.1911d}$$
$$(8c)$$

$$T_{det} = 298 + \frac{\Delta H_f(c) + 625.2a - 142.8b}{59.05 \times 10^{-3}a - 43.81 \times 10^{-3}b} \quad (8d)$$
$$+18.66 \times 10^{-3}c + 20.36 \times 10^{-3}d$$

where T_{det} is detonation temperature in K and $\Delta H_f(c)$ is the condensed phase heat of formation of explosive in kJ/mol.

Detonation temperature of $C_aH_bN_cO_d$ explosives can be predicted from elemental composition and the calculated gas phase heat of formation of explosives without using any assumed detonation products and experimental data. It was shown that two correlations can be used for calculation of detonation temperature of aromatic and non-aromatic explosive compounds. The following correlations can be obtained for aromatic and non-aromatic explosives, respectively [29]:

$$\frac{T_{det}}{1000} = -75.8 + \left(\frac{950.8a + 12.3b + 1115c + 1324d + 1.2\Delta H_f(g)}{MW} \right) \quad (9a)$$

$$\frac{T_{det}}{1000} = 149.0 + \left(\frac{-1514a - 196.5b - 206.6c - 2346d + 1.2\,\Delta H_f(g)}{MW} \right) \quad (9b)$$

These equations provide a simple procedure for estimation of detonation temperature of explosives, which require as input information only the elemental composition and the calculated gas phase heat of formation of the explosive by Joback's method [22,23].

2.4. Adiabatic exponent

A general reliable simple equation can be used for prediction of the adiabatic exponent of explosives at any loading density as a parameter used to describe the detonation isentrope [30]. It is in turn as a criterion for selecting detonation pressure of explosives from among experimental measurement especially for loading density less than $1.0\,g/cm^3$. However, it can be given as:

$$\gamma = 1.819 - \frac{0.196}{\rho_0} + 0.712\rho_0 \quad (10)$$

2.5. Energy output and Gurney velocity of explosives

Gurney [31] introduced a simple model in which a given explosive librates a fixed amount of specific energy on detonation that is converted to kinetic energy partitioned between the driven metal and gaseous products. Two correlations [32] were recently introduced for calculating Gurney velocity ($\sqrt{2E}$) in which only the chemical composition of high explosive as well as its condensed or estimated gas phase heat of formation by Joback's method [22,23] can be used. They may be applied to any explosive that contains carbon, hydrogen, nitrogen and oxygen atoms without using any assumed decomposition reactions. The following correlations can be used for reliable calculating Gurney velocity by using condensed and gas phase heat of formation of explosive, respectively:

$$\sqrt{2E} = 0.227 + \left(\frac{\begin{array}{c} 7.543a + 2.676b + 31.97c \\ +35.91d - 0.196\,\Delta H_f(c) \end{array}}{MW} \right) \rho_0^{0.5} \quad (11)$$

$$\sqrt{2E} = 0.220 + \left(\frac{\begin{array}{c} 6.620a + 4.427b + 29.03c \\ +37.61d - 0.051\Delta H_f(g) \end{array}}{MW} \right) \rho_0^{0.5} \quad (12)$$

where $\sqrt{2E}$ is in km/s.

2.6. Specific impulse

The specific impulse can be used to characterize the propellant performance. It can be defined as the thrust divided by the propellant consumption rate. A high explosive can be designated as a monopropellant that its specific impulse depends upon chemical and structural factor. A simple method can be used to estimate specific impulse of mostly ideal and less ideal composition explosives by detonation velocity of explosive, which can be designated as a monopropellant, and loading density. The simple empirical equation has the form [33]:

$$I_{SP} = \frac{D - 1.98}{1.453\rho_0} \quad (13)$$

where I_{SP} is the specific impulse (in N s/g).

2.7. Detonation velocity and pressure in aluminized explosives

Non-ideal explosives can have the C-J detonation pressure and velocity significantly different from those expected by a computer code such as BKW for equilibrium and steady-state calculations [1]. Aluminized composite explosives are well-known non-ideal explosives in which finely dispersible aluminum powders can be used in explosives to increase their performances. Detonation velocity and pressure can be calculated through thermochemical/hydrodynamic computer codes such as BKW [1] by assuming a certain degree of aluminum oxidation because its value in the C-J point for mixture of high explosives with aluminum is not clear. Detonation velocity and pressure for aluminized explosives with general formula $C_aH_bN_cO_dAl_e$ can be given as follows [34,35]:

$$D = -0.5823a + 0.2335b + 0.0976c + 0.3041d$$
$$-1.1090e + 4.5201\rho_0 \quad (14)$$

$$P = -35.531a + 41.422b - 14.770c + 44.004d$$
$$-21.320e + 43.950\rho_0^2 \quad (15)$$

The temperature and energy released by aluminized explosives are sensitive to the degree of aluminum reaction because aluminum can react with the gaseous products CO_2, H_2O and CO of detonation in exothermic reactions. The main result of increased heat is a prolongation of the pressure effect. Aluminum, being a non-explosive substance in itself, takes an appreciable time to react, and therefore reduces the velocity of detonation. The predicted detonation pressure and velocity in Eqs. (14) and (15) are consistent with increasing the percentage of aluminum [34,35].

3. Computation of performance and thermochemical properties of energetic materials by EDPHT

The algorithm of EDPHT in prediction of performance and thermochemical properties of pure and composite mixture of high explosives as well as detonation velocity and pressure in aluminized explosives is shown in Fig. 1 as flow chart. The software EDPHT can predict various properties of $C_aH_bN_cO_d$ high explosives including velocity of detonation, detonation pressure, heat of detonation, detonation temperature, Gurney velocity, adiabatic

exponent and specific impulse. If the condensed phase heat of formation of an energetic compound is not available, EDPHT can predict ΔH_f(g) through its molecular structure by Joback's method [22,23]. For composite mixture of high explosives, only mass percent of different components as well as their molecular formulas and structures may be needed as input parameters.

The software EDPHT based on computational technique is developed to run on windows operating system. Visual Basic 6.0 was chosen as an efficient application tool to develop this numerical modeling software. This software occupies about 12.3 MB of hard disk space in the computer and its output can be directly printed. Loading density, empirical formula and molecular structure can be used as input parameters to predict mentioned performance and thermochemical properties of energetic materials. Since detonation pressure of explosives strongly depends on its loading density, some recent methods can be used for prediction density of novel non-aromatic, polynitro arene and heteroarene energetic compounds [36,37].

4. Results and discussion

4.1. Prediction of gas phase heat of formation

Different group additivity methods can be used to estimate the standard-state enthalpy of formation for organic compounds in the ideal-gas standard state [15]. Of various methods, Joback's method [22,23] is a very simple method. It requires two-dimensional molecular structures of desired organic molecules. It assigns contributions to common molecular groupings, e.g., $-CH_3$, $-NH_2-$, $-COOH$, which are simply added. The following equation can be used to gas phase heat of formation on the basis of the Joback's method:

$$\Delta H_f^{\circ}(298.15\,\text{K}) = 68.29 + \sum n_i \delta_i \qquad (16)$$

where n_i and δ_i are the number and contribution of the ith atomic or molecular group, respectively. Poling et al. [15] have shown that the Joback's method [22,23] is marginally accurate for the formation properties of all substances regardless of size. The EDPHT can predict gas phase enthalpy of formation of an explosive through typing the number of specific atoms and molecular groups in definite input data sheet as a look-up table on the basis of molecular fragments corresponding to molecular structure.

4.2. Validation of EDPHT by well-known explosives and comparison of the predicted results with the other computer codes

The predicted results of EDPHT for performance and thermochemical properties of various $C_aH_bN_cO_d$ can be compared with outputs of the other computer codes. The computational approaches in EDPHT can also be validated by comparing the predicted values with the experimentally determined results reported in the literature. For calculation of different parameters, twelve examples of well-known explosives ranging from oxygen lean to rich compounds were selected for each case. The explosives in tables cover a wide range in oxygen balance and are considered to be representative of the entire class of CHNO explosives. For example, NG has more than enough oxygen in its structure to oxidize fully the fuel elements of the molecule; on the other hand, TNT is very oxygen deficient because some carbon is not been oxidized. The other explosives in Tables have oxygen content between NG and TNT. Moreover, among various $C_aH_bN_cO_d$ explosives, PETN can be prepared in high purity and pressed into manageable charges over a wide range of density that make it an ideal explosive for testing theoretical models. Further examples for the introduced equations in section two can be found in corresponding references. Difference of predictions from experiments, e.g. Dev = measured-predicted, for various desired performance and thermochemical properties of energetic compounds are given in corresponding tables. The root mean square (rms) of deviations also given in different tables, which can be defined as:

$$\text{rms deviation} = \sqrt{\frac{1}{N}\sum_{j=1}^{N}\text{Dev}_j^2} \qquad (17)$$

where N represents the number of measurements.

The experimentally determined values of heats of detonation for some energetic compounds, with the H_2O in liquid state, and the predicted results using EDPHT and LOTUSES are presented in Table 1. As seen in Table 1, the predicted results for both codes are close to each other. Both codes, which are based on different empirical methods, show good agreement with experimental values as indicated in Table 1. However, EDPHT can be applied for a wide range of explosives including under-oxidized and over-oxidized explosives. The rms of deviations predicted by EDPHT on the basis of ΔH_f (c) of energetic compound is lower than those reported by LOTUSES. The rms of deviations of the results by EDPHT on the basis of ΔH_f (g) is slightly higher than LOTUSES.

Detonation velocities estimated by EDPHT and LOTUSES as well as BKWR-EOS and BKWS-EOS for under-oxidized and over-oxidized explosives are given in Table 2 and compared with the measured values. Since LOTUSES is based on the empirical method of Rothstein and Petersen [38,39], which introduces a simple relationship between detonation velocity at theoretical maximum density and chemical composition, only the highest experimental detonation velocities at large loading density are given in Table 2. As indicated in Table 2, EDPHT has the lowest rms value with respect

Table 1
Comparison of the calculated heats of detonation (kJ/g) by EDPHT, on the basis of gas and condensed phase heat of formation of energetic compound, and LOTUSES [14] with the measured values [40].

| Explosive	Exp.	EDPHT (ΔH_f (g))	Dev	EDPHT (ΔH_f (c))	Dev	LOTUSES	Dev
BTNEU	6.454	7.27	−0.82	6.49	−0.04	6.38	0.07
DINA	5.458	5.57	−0.11	5.46	0.00	5.02	0.44
DIPEHN	5.143	5.72	−0.58	5.15	−0.01	4.81	0.33
EDNA	4.699	4.71	−0.01	4.6	0.10	5.18	−0.48
Ethriol trinitrate	4.244	4.81	−0.57	3.87	0.37	3.73	0.51
MHN	6.384	7.04	−0.66	6.35	0.03	5.94	0.44
Nitromethane	4.821	4.82	0.00	4.65	0.17	4.72	0.10
Nitrourea	3.745	4.53	−0.79	3.79	−0.04	3.65	0.10
PETN	6.322	6.32	0.00	6.35	−0.03	6.13	0.19
PETRIN	5.230	5.37	−0.14	5.24	−0.01	4.70	0.53
RDX	6.322	6.28	0.04	5.66	0.66	5.09	1.23
TETRYL	4.773	3.69	1.08	3.76	1.01	4.53	0.24
rms deviation (kJ/g)			0.55		0.37		0.49
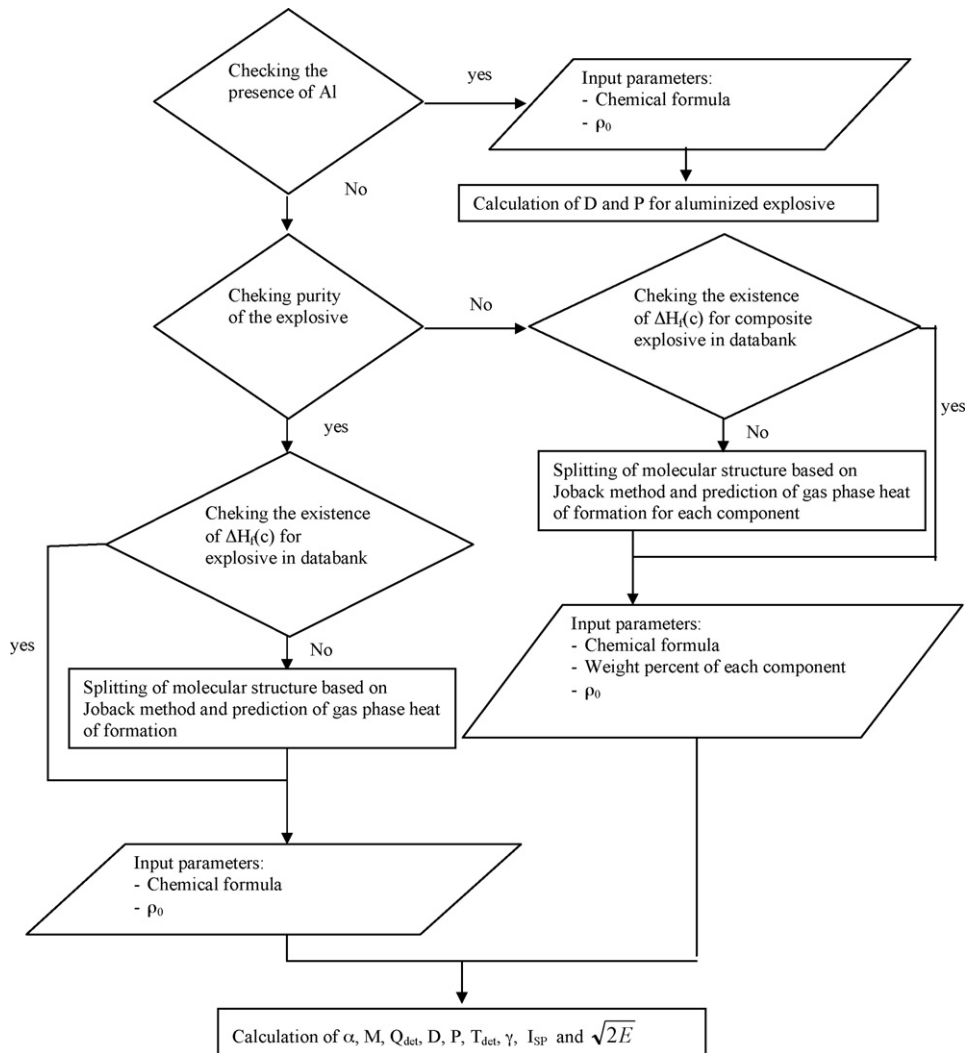
Fig. 1. Block diagram of the software EDPHT.

to the predicted results of the other computer codes. Since EDPHT is based on recent correlations that provide small errors in predictions at initial densities less than $1 \, \text{g/cm}^3$, it can determine detonation velocity to within about few percent at any loading density. Thus, the agreement between calculated values and measured velocities in Table 2 is good because errors of a few percent can generally be attributed to measurements of detonation velocity.

The predicted detonation pressures by the new computer code and outputs of the other computer codes for the same explosives are given in Table 3 and compared with corresponding measured values. As seen, the same as detonation velocity, the predicted results by EDPHT has the lowest rms value which show good agreement with experimental values. Since large deviations generally attributed to experimental measurements of detonation pressure

Table 2
Comparison of the calculated detonation velocity (km/s) by EDPHT, on the basis of gas and condensed phase heat of formation of energetic compound, BKWR-EOS [9], BKWS-EOS [9] and LOTUSES [11] with the measured values [9].

Explosive	ρ_0 (g/cm^3)	Exp.	EDPHT (ΔH_f(g))	Dev	EDPHT (ΔH_f(c))	Dev	BKWR	Dev	BKWS	Dev	LOTUSES	Dev
COMP B-3	1.72	7.89	7.98	−0.09	8.05	−0.16	8.08	−0.19	8.16	−0.27	7.93	−0.04
CYCLOTOL-77/23	1.74	8.25	8.28	−0.03	8.27	−0.02	8.33	−0.08	8.44	−0.19	8.31	−0.06
DATB	1.80	7.60	7.60	0.00	7.63	−0.03	7.92	−0.32	7.86	−0.26	7.69	−0.09
HMX	1.89	9.11	9.09	0.02	8.98	0.13	9.08	0.03	9.35	−0.24	9.04	0.07
NG	1.60	7.70	7.91	−0.21	7.87	−0.17	7.94	−0.24	8.01	−0.31	7.25	0.45
OCTOL-76/23	1.81	8.45	8.49	−0.04	8.46	−0.01	8.54	−0.09	8.70	−0.25	8.59	−0.14
PETN	1.76	8.27	8.27	0.00	8.48	−0.21	8.23	0.04	8.67	−0.40	8.08	0.19
RDX	1.80	8.75	8.81	−0.06	8.65	0.10	8.77	−0.02	8.96	−0.21	8.93	−0.18
TATB	1.88	7.76	7.73	0.03	7.72	0.04	8.28	−0.52	8.19	−0.43	7.86	−0.10
TETRYL	1.73	7.72	7.73	−0.01	7.92	−0.20	7.75	−0.03	7.81	−0.09	7.77	−0.05
TNM	1.64	6.36	6.63	−0.27	6.48	−0.12	6.22	0.14	5.54	0.82	8.26	−0.39
TNT	1.64	6.93	6.94	−0.01	7.19	−0.26	7.20	−0.27	7.19	−0.26	6.66	0.27
rms deviation (km/s)				0.11		0.14		0.22		0.36		0.21

Table 3
Comparison of the calculated detonation pressure (GPa) by EDPHT, on the basis of gas and condensed phase heat of formation of energetic compound, BKWR-EOS [9], BKWS-EOS [9] and LOTUSES [11] with the measured values [9].

Explosive	ρ_0 (g/cm^3)	Exp.	EDPHT (ΔH_f(g))	Dev	EDPHT (ΔH_f(c))	Dev	BKWR	Dev	BKWS	Dev	LOTUSES	Dev
COMP B-3	1.72	28.7	27.5	1.20	28.7	0.00	29.9	−1.20	27.3	1.40	28.4	0.30
CYCLOTOL-77/23	1.74	31.1	30.3	0.80	30.9	0.20	32.0	−0.90	29.4	1.70	31.3	−0.20
DATB	1.80	25.1	25.3	−0.20	24.7	0.40	29.2	−4.10	25.8	−0.70	27.8	−2.70
HMX	1.89	39.0	39.0	0.00	38.4	0.60	40.5	−1.50	37.4	1.60	39.5	−0.50
NG	1.60	25.3	28.5	−3.20	26.9	−1.60	26.0	−0.70	25.0	0.30	22.0	3.30
OCTOL-76/23	1.81	33.8	32.6	1.20	33.2	0.60	35.0	−1.20	32.1	1.70	34.4	−0.60
PETN	1.76	33.7	32.2	1.50	33.0	0.70	29.8	3.90	31.2	2.50	29.6	4.10
RDX	1.80	34.1	35.5	−1.40	34.8	−0.70	36.4	−2.30	33.4	0.70	37.3	−3.20
TATB	1.83	26.0	28.8	−2.80	23.8	2.20	31.4	−5.40	27.1	−1.10	30.2	−4.20
TETRYL	1.71	23.9	23.9	0.00	26.8	−2.90	27.0	−3.10	24.8	−0.90	27.1	−3.20
TNT	1.64	21.0	18.4	2.60	20.8	0.20	22.3	−1.30	20.3	0.70	19.2	1.80
TNM	1.64	15.9	16.4	−0.50	15.3	0.60	15.0	0.90	11.6	4.30	19.5	−3.60
rms deviation (GPa)				1.65		1.23		2.66		1.79		2.74

[1], the agreement between outputs of different computer codes and measured pressures is also satisfactory.

The predicted detonation temperatures for explosives are given in Table 4 and compared with corresponding measured values and computed results by BKWR-EOS and BKWS-EOS. Some of the calculated values by simple computer code LOTUSES are also given in Table 4. As seen, EDPHT on the basis of the condensed phase heat of formation of explosive provides the lowest rms value. It should be mentioned that by considering large deviations generally attributed to experimental measurements of detonation tempera-

ture, the agreement between calculated and measured values in all of computer codes are also satisfactory.

Since condensed explosives of practical interest have loading densities in the range 0.2–2 g/cm^3, EDPHT can provide good results with properties in the C-J state and loading density in this range. Adiabatic exponent is strongly dependent on the loading density and only a very weak function of the exact chemical composition of the explosive. Computed adiabatic exponent of explosives by EDPHT are given in Table 5 and compared with corresponding measured values as well as computed results of BKWR-EOS

Table 4
Comparison of the calculated detonation temperature (K) by EDPHT, on the basis of gas and condensed phase heat of formation of energetic compound, BKWR-EOS [9], BKWS-EOS [9] and LOTUSES [11] with the measured values [9].

Explosive	ρ_0 (g/cm^3)	Exp.	EDPHT (ΔH_f(g))	Dev	EDPHT (ΔH_f(c))	Dev	BKWR	Dev	BKWS	Dev	LOTUSES	Dev
COMP B-3	1.72		3918		4072		3260		4000			
CYCLOTOL-77/23	1.74		4032		3947		3260		4070			
DATB	1.80		3643		3506		2860		3550			
HMX	1.60	4300	4162	138	4297	3	3470	830	4270	30	4500	−200
NG	1.60	4260	3656	604	4259	1	3750	510	4550	−290	4500	−240
OCTOL-76/23	1.81		3974		3938		3170		4020			
PETN	1.60	4400	4161	239	4401	−1	3520	880	4390	10	5000	−600
RDX	1.66	4320	4184	136	4433	−113	3400	920	4230	90	4500	−180
	1.40	4610	4184	426	4433	177	3690	920	4390	220	4500	110
	1.20	4610	4184	426	4433	177	3840	770	4460	150	4500	110
	1.00	4600	4184	416	4433	167	3920	680	4490	110	4500	100
TATB	1.88		3418		3251		2550		3250			
TETRYL	1.61	4200	3987	213	4253	−53	3590	610	4270	−70		
	1.40	4130	3987	143	4253	−123	3750	380	4350	−220		
	1.20	4300	3987	313	4253	47	3840	460	4380	−80		
TNM	1.64	2800	3178	−378	2590	210	2180	620	2860	−60		
TNT	1.00	3400	3511	−111	3401	−1	3410	−10	3750	−350	2800	600
rms deviation (K)				331		118		682		174		332

Table 5
Comparison of the calculated adiabatic exponent by EDPHT, BKWR-EOS [9] and BKWS-EOS [9] with the measured values [9].

Explosive	ρ_0 (g/cm^3)	Exp.	EDPHT	Dev	BKWR	Dev	BKWS	Dev
COMP B-3	1.72	2.73	2.93	−0.20	2.76	−0.02	3.20	−0.46
CYCLOTOL-77/23	1.74	2.78	2.95	−0.16	2.77	0.01	3.22	−0.43
DATB	1.80	3.14	2.99	0.15	2.87	0.27	3.31	−0.17
HMX	1.89	3.02	3.06	−0.04	2.85	0.17	3.42	−0.40
NG	1.60	2.75	2.84	−0.09	2.88	−0.13	3.11	−0.36
OCTOL-76/23	1.81	2.82	3.00	−0.18	2.77	0.05	3.27	−0.44
PETN	1.76	2.57	2.96	−0.39	3.00	−0.43	3.24	−0.67
RDX	1.80	3.04	2.99	0.05	2.80	0.24	3.33	−0.29
TATB	1.85	3.19	3.03	0.16	2.94	0.25	3.45	−0.25
TETRYL	1.68	2.95	2.9	0.05	2.73	0.22	3.09	−0.14
TNM	1.64	3.17	2.87	0.30	3.23	−0.06	3.34	−0.17
TNT	1.64	2.75	2.87	−0.12	2.81	−0.06	3.18	−0.43
rms deviation				0.19		0.20		0.38

Table 6
Comparison of the calculated Gurney velocity (km/s) by EDPHT, on the basis of gas and condensed phase heat of formation of energetic compound, with the measured values [32].

Explosive	ρ_0 (g/cm^3)	Exp.	EDPHT (ΔH_f (g))	Dev	EDPHT (ΔH_f (c))	Dev
COMP B-3	1.72		2.68		2.68	
CYCLOTOL-77/23	1.74	2.79	2.76	0.03	2.76	0.03
DATB	1.80		2.60		2.65	
HMX	1.89	2.97	2.97	0.0	2.97	0.0
NG	1.60		2.86		2.86	
OCTOL-76/23	1.81		2.81		2.81	
PETN	1.76	2.93	2.93	0.0	2.93	0.0
RDX	1.77	2.88	2.88	0.0	2.88	0.0
TATB	1.83		2.67		2.74	
TETRYL	1.62	2.50	2.50	0.0	2.50	0.0
TNM	1.64		3.00		2.97	
TNT	1.63	2.37	2.37	0.0	2.37	0.0
rms deviation (km/s)				0.01		0.01

Table 7
Comparison of the calculated specific impulse (N s/g) by EDPHT, on the basis of gas and condensed phase heat of formation of energetic compound, with the computer code ISPBKW [1].

Explosive	ρ_0 (g/cm^3)	Exp.	EDPHT (ΔH_f (g))	Dev	EDPHT (ΔH_f (c))	Dev
COMP B-3	1.72	2.434	2.40	0.03	2.428816	0.01
CYCLOTOL-77/23	1.74	2.508	2.49	0.02	2.487916	0.02
DATB	1.80	2.139	2.15	−0.01	2.160281	−0.02
HMX	1.89	2.614	2.59	0.02	2.549005	0.06
NG	1.60	2.285	2.55	−0.27	2.533551	−0.25
OCTOL-76/23	1.81	2.500	2.48	0.02	2.463944	0.04
PETN	1.76	2.596	2.46	0.14	2.541763	0.05
RDX	1.80	2.618	2.61	0.01	2.550279	0.07
TATB	1.88	2.006	2.10	−0.10	2.101302	−0.10
TETRYL	1.73	2.50	2.29	0.21	2.36306	0.14
TNM	1.64	1.900	1.95	−0.05	1.888439	0.01
TNT	1.64	2.102	2.08	0.02	2.186393	−0.08
rms deviation (N s/g)				0.11		0.10

Table 8
Comparison of the calculated detonation velocity (km/s) of aluminized explosives by EDPHT and BKWS-EOS (using full and partial, 50%, interaction of aluminum with detonation products) with measured values [9].

Explosive	ρ_0 (g/cm^3)	Exp.	EDPHT	Dev	BKWS-EOS (FULL)	Dev	BKWS-EOS (PARTIAL)	Dev
Alex 20	1.801	7.53	7.59	−0.06				
Alex 32	1.88	7.30	7.42	−0.12				
Destex	1.68	6.65	6.44	0.21				
HBX-1	1.72	7.22	7.32	−0.10	7.18	0.04	7.38	−0.16
HMX/Al (90/10)	1.76	8.30	8.38	−0.08	8.32	−0.02	8.41	−0.11
HMX/Al (60/40)	1.94	7.70	7.68	0.02	6.86	0.84	7.46	0.24
PBXN-1	1.77	7.93	7.77	0.16				
RDX/Al (90/10)	1.68	8.03	8.02	0.01	8.02	0.01	8.08	−0.05
RDX/Al (60/40)	1.84	7.20	7.23	−0.03	6.42	0.78	6.93	0.27
TNETB/Al (90/10)	1.75	8.12	8.14	−0.02	7.85	0.27	7.91	0.21
TNETB/Al (70/30)	1.88	7.84	7.77	0.07	6.99	0.85	7.43	0.41
TNT/Al (78.3/21.7)	1.8	7.05	6.97	0.08	6.59	0.46	6.94	0.11
rms deviation (km/s)				0.10		0.54		0.22

Table 9
Comparison of the calculated detonation pressure (GPa) of aluminized explosives by EDPHT and BKWS-EOS (using full and partial, 50%, interaction of aluminum with detonation products) with measured values [9].

Explosive	ρ_0 (g/cm^3)	Exp.	EDPHT	Dev	BKWS-EOS (full)	Dev	BKWS-EOS (partial)	Dev
Alex 20	1.801	23.0	22.8	0.20				
Alex 32	1.88	21.5	21.6	−0.10				
Destex	1.68	17.5	17.8	−0.30				
HBX-1	1.71	22.0	21.8	0.20	21.1	0.90	20.9	1.10
HMX/Al (90/10)	1.76		25.7		29.1		28.5	
HMX/Al (60/40)	1.94		22.0		18.0		20.4	
PBXN-1	1.77	24.5	24.5	0.00				
RDX/Al (90/10)	1.68	24.6	24.5	0.10	26.4	−1.80	25.7	−1.10
RDX/Al (60/40)	1.84	21.1	20.3	0.80	15.6	5.50	17.4	3.70
TNETB/Al (90/10)	1.75	26.2	25.8	0.40	26.9	−0.70	25.8	0.40
TNETB/Al (70/30)	1.88	22.7	23.4	−0.70	21.9	0.80	21.9	0.80
TNT/Al (78.3/21.7)	1.8	18.9	18.7	0.20	18.3	0.60	18.7	0.20
rms deviation (GPa)				0.39		2.44		1.68

Table 10

Comparison of the calculated detonation pressure and velocity for various explosives (including solid one component, solid mixture and liquids) with $C-NO_2$, $O-NO_2$ and $N-NO_2$ energetic groups by EDPHT, BKW TNT parameter and BKW RDX parameter.

Explosive	ρ_0 (g/cm³)	Experimental		BKW TNT parameter				BKW RDX parameter				EDPHT			
		D (km/s)	P (GPa)	D (km/s)	Dev	P (Gpa)	Dev	D (km/s)	Dev	P (Gpa)	Dev	D (km/s)	Dev	P (Gpa)	Dev
ABH	1.78	7.6		7.34	0.26	25.4		7.63	−0.03	26.5		7.97	−0.37	27.9	
ANFO	0.88	5.5						5.44	0.06	73.4		5.05	0.45	6.5	
1/1.29 moles benzene/tetranitromethane	1.362	6.85						6.96	−0.11	18.1		6.95	−0.1	18.9	
Cyclotol 77/23	1.743	8.25	31.3	7.91	0.34	28.8	2.5	8.31	−0.06	30.5	0.8	8.27	−0.02	30.9	0.4
Comp. B 64/36	1.713	8.03	29.4					8.08	−0.05	28.4	1	8.06	−0.03	28.7	0.7
DATB	1.788	7.52	25.9	7.56	−0.04	26.4	−0.5	7.96	−0.44	28.2	−2.3	7.77	−0.25	25.9	0
DIPAM	1.79	7.5		7.38	0.12	25.5		7.74	−0.24	26.9		7.8	−0.3	26.2	
EDC-11	1.782	8.12	31.5					8.38	−0.26	32.5	−1	8.29	−0.17	31.1	0.4
EDC-24	1.776	8.71	34.2					8.64	0.07	33.4	0.8	8.47	0.24	32.9	1.3
Explosive D	1.55	6.85						6.99	−0.14	18.9		6.66	0.19	16.6	
HMX	1.9	9.1	39.3	9.16	−0.06	39.5	−0.2	8.56	0.54	36.4	2.9	9.01	0.09	38.8	0.5
75/25 HMX/HYDRAZINE	1.86	9.1						9.24	−0.14	38.8		8.9	0.2	37.6	
6.435/2.2275/6.435 moles $HNO_3/H_2O/CH_3NO_2$	1.29	6.54	14.5					6.67	−0.13	15.3	−0.8	6.55	−0.01	15.8	−1.3
HNS	1.74	7.13		7.13	0	23.1		7.41	−0.28	24.1		7.59	−0.46	24.3	
LX-14	1.81	8.76						8.75	0.01	34.8		8.63	0.13	34.6	
NG	1.59	7.58						7.70	−0.12	24.6		7.85	−0.27	26.7	
Nitromethane	1.128	6.29	14.1	6.39	−0.1	13.0	1.1	6.46	−0.17	13.0	1.1	6.2	0.09	13.3	0.8
1/0.071 moles nitromethane/tetranitromethane	1.197	6.57	13.8					6.80	−0.23	15.3	−1.5	6.52	0.05	15.6	−1.8
1/0.25 moles nitromethane/tetranitromethane	1.31	6.88	15.6					7.09	−0.21	18.1	−2.5	7.03	−0.15	19.5	−3.9
1/0.5 moles nitromethane/tetranitromethane	1.397	6.78	16.8					6.91	−0.13	17.9	−1.1	7.02	−0.24	19.4	−2.6
NONA	1.78	7.56		7.27	0.29	24.9		7.57	−0.01	26.0		7.89	−0.33	27.1	
OCTOL-76.3/23.7	1.809	8.48	34.3					8.56	−0.08	33.3	1	8.5	−0.02	33.2	1.1
ONT	1.8	7.33		7.25	0.08	24.7		7.56	−0.23	26.0		7.79	−0.46	26.2	
PBX-9011	1.767	8.5	29.8					8.50	0	31.9	−2.1	8.4	0.1	32.2	−2.4
PBX-9501	1.841	8.83						8.89	−0.06	36.3		8.76	0.07	36.0	
PBXC-116	1.65	7.96						7.93	0.03	25.8		7.47	0.49	23.2	
PBX-119	1.635	8.08						8.13	−0.05	27.4		7.89	0.19	27.1	
PENTOLITE	1.65	7.47		7.47	0	24.7		7.74	−0.27	25.7		7.82	−0.35	26.5	
PETN	1.67	7.98	30.0	7.70	0.28	26.7	3.3	8.06	−0.08	28.0	2	8.14	−0.16	29.5	0.5
	1.77	8.3	33.5					8.42	−0.12	31.8	1.7	8.51	−0.21	33.3	0.2
	1	5.48	8.7					5.95	−0.47	10.1	−1.4	5.66	−0.18	9.9	−1.2
	0.5	3.6	2.4					4.31	−0.71	3.03	−0.63	3.82	−0.22	1.6	0.8
95/5 PYX/polyethylene	1.556	7.1						6.90	0.2	18.8		6.94	0.16	18.8	
RDX	1.8	8.75	34.7	8.26	0.49	32.4	2.3	8.75	0	34.7	0	8.65	0.1	34.8	−0.1
	1	5.98						6.13	−0.15	10.8		5.68	0.3	10.0	
Z-TACOT	1.85	7.25		7.43	−0.18	26.3		7.76	−0.51	27.8		7.85	−0.6	26.7	
TATB	1.895	7.86	31.5	7.85	0.01	29.7	1.8	8.41	−0.55	32.6	−1.1	7.73	0.13	25.6	5.9
Tetryl	1.7	7.56						7.63	−0.07	25.1		7.72	−0.16	25.5	
TNT	1.64	6.95	19.0	6.95	0	20.6	−1.6	7.20	−0.25	21.3	−2.3	7.16	−0.21	20.6	−1.6
	1.061	5.25	11.0	5.34	−0.09	8.5	2.5					5.33	−0.08	8.0	3
	0.732	4.2	5.9	4.51	−0.31	4.5	1.4					4.3	−0.1	3.2	2.7
TNT (liquid)	1.447	6.58	17.2	6.41	0.17	15.7	1.5	6.56	0.02	16.0	1.2	6.59	−0.01	16.1	1.1
14.5/85.5 toluene/nitromethane	1.088	5.84	10.0					5.95	−0.11	10.6	−0.6	5.58	0.26	9.4	0.6
rms deviation[a]				0.21		1.9		0.25		1.7		0.24		1.9	

[a] For detonation pressure and velocity are in GPa and km/s, respectively.

and BKWS-EOS. As indicated, EDPHT gives good predictions with respect to complex computer outputs.

Gurney velocities estimated by EDPHT are given in Table 6 and compared with measured values. As indicated in Table 6, the new computer code shows good agreement with experimental values at specified loading densities. It is seen that the predicted results approximates the measured results most closely because predicted Gurney velocities for 12 explosives by using both the condensed and gas phase heats of formation have a rms of deviations for experiment 0.01 km/s. Computed Gurney velocities by EDPHT are insensitive to large variation in the heat of formation of unreacted explosive. Thus, the contribution of the four elements present in explosive as input parameters of the computer code is far more important, in terms of influencing Gurney velocity, than details of the bonding arrangements within the molecular structure. There are individual compounds such as TNT, RDX and PETN in Table 6 which have $C–NO_2$, $N–NO_2$ and $O–NO_2$ bonds, respectively.

Specific impulse of various explosives given in Table 7 are calculated and compared with computed values of ISPBKW computer code [1]. As seen, deviations of predicted values of EDPHT from ISP-BKW computer code for pure and composite explosives are small. This comparison may be taken as appropriate validation test of the new method for high explosives. Although ISPBKW computer code is a complex computer code, the new computer code EDPHT provides specific impulse of high explosives simply by considering them as monopropellants.

An ideal explosive can be described adequately for engineering purpose by steady-state detonation calculations using appropriate equations of state. Some explosives like HMX, RDX and TNT should have short reaction zone and have small failure diameters, which are suitable for practical applications. Since aluminized explosives have significantly different detonation properties than those predicted, they can be considered as non-ideal explosives. Computed detonation velocities and pressures of some aluminized explosives are given in Tables 8 and 9. To use EDPHT for aluminized explosives, 100 g of aluminized explosives should be taken for calculation of detonation velocity and pressure. As shown in Tables 8 and 9, the computed detonation velocities and pressures of aluminized explosives are also compared with BKWS-EOS using full and partial equilibrium of Al. In the case of partial equilibrium, only 50% of aluminum is assumed to interact with combustion products. As indicated in Tables 8 and 9, EDPHT shows the lowest rms value with respect to the computed results of complicated computer program. The EDPHT requires no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical property of explosive and assumed detonation products.

4.3. Comparison of the possible data with BKW computer code

The BKW-EOS is an equation of state extensively used to calculate detonation properties. Mader [1] gives the molecular covolumes for the BKW-EOS in the following form:

$$\frac{PV}{RT} = 1 + Xe^{\beta X} \text{ with } X = \frac{\kappa \sum x_i k_i}{VT^{0.5}} \tag{18}$$

where P, V, R, T and x_i represent pressure, molar gas volume, gas constant, absolute temperature and mole fraction of the ith gaseous component, respectively. The summation extends over all components of the gaseous mixture. The covolume factors, k_i, represent excluded volume. The values β and κ are empirical constants. The parameters β, κ and k_i can be adjusted to fit measured detonation properties. The BKW code is the most and best calibrated of those used to calculate detonation properties assuming steady-state and chemical equilibrium. It should be noted that two parameter sets can be used to calculate detonation performance by the BKW com-

puter code. The RDX parameter can be used for most explosives and the TNT parameter set can be applied for those explosives with large amounts of carbon in the detonation products.

For CHNO explosives, where measured detonation pressure and velocity were available, we can compare predicted results by complex computer code BKW with simple code EDPHT. The predicted outputs for these detonation parameters on the basis of BKW RDX and TNT parameters are given in Table 10. As indicated in Table 10, the calculated results for both codes are relatively close to each other.

There are some advantages and some drawbacks or demerits of the presently developed code in comparison to internationally acclaimed codes such as BKW.

Advantages:

(a) This code can complemented the computer outputs of the other thermodynamic chemical equilibrium codes.
(b) The EDPHT not only provides important information about detonation performance but also some new aspects of explosives (e.g. Gurney velocity) simultaneously.
(c) The new computer code is very simple for user and requires minimum input data.
(d) There is no need to use RDX and TNT parameters for which different values of detonation parameters can be predicted for the same explosive.

Disadvantages:

(a) The new code can be applied only to CHNO explosives. It cannot be used for the other explosives with further elements, e.g. halogens.
(b) The calculated data on the basis of the condensed phase heat of formation is more reliable than gas phase heat of formation of explosive. Thus, it is better to use approximate condensed phase heat of formation.
(c) The parameter particle size cannot be considered in the new code, the same as the other well-known computer codes, during the performance prediction of energetic materials.

5. Conclusions

A simple computer code (EDPHT) complemented the outputs of the other computer codes has been introduced to predict velocity of detonation, detonation pressure, heat of detonation, detonation temperature, Gurney velocity, adiabatic exponent and specific impulse of high explosives with general formula $C_aH_bN_cO_d$. This code can also be used to predict detonation velocities and pressures of aluminized explosives, which have general formula $C_aH_bN_cO_dAl_e$. The EDPHT does not require using full or partial oxidation of aluminum that is usually required by the other thermochemical/hydrodynamic computer codes. To validate the developed code, large amount of data of different classes of explosives from $C–NO_2$, $O–NO_2$ and $N–NO_2$ groups have been generated.

Appendix A. Glossary of compound names for pure as well as composite explosives on the basis of 100 g for mixture of different compounds

1. ABH: azobis(2,2′,4,4′,6,6′-hexanitrobiphenyl) ($C_{24}H_6N_{14}O_{24}$)
2. Alex 20: $C_{1.783}H_{2.469}N_{1.613}O_{2.039}Al_{0.7335}$
3. Alex 32: $C_{1.647}H_{2.093}N_{1.365}O_{1.744}Al_{1.142}$

4. ANFO: 6/94 oil/ammonium nitrate ($C_{0.365}H_{4.7129}N_2O_3$)
5. 1/1.29 moles benzene/tetranitromethane ($C_{7.29}H_6N_{5.16}O_{10.32}$)
6. BTNEU: bi-trinitroethylurea ($C_5H_6N_8O_{13}$)
7. COMP B: 64/36 RDX/TNT ($C_{6.851}H_{8.750}N_{7.650}O_{9.3}$)
8. COMP B-3: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
9. CYCLOTOL-77/23: 77/23 RDX/TNT ($C_{1.75}H_{2.59}N_{2.38}O_{2.69}$)
10. DATB: 1,3-diamino-2,4,6-trinitrobenzene ($C_6H_5N_5O_6$)
11. Destex: $C_{2.791}H_{2.3121}N_{0.987}O_{1.975}Al_{0.6930}$
12. DINA: dioxyethylnitramine dintrate ($C_4H_8N_4O_8$)
13. DIPAM: dipicramide ($C_{12}H_6N_8O_{12}$)
14. DIPEHN: dipentaerythritol hexanitrate ($C_{10}H_{16}N_6O_{19}$)
15. EDC-11:64/4/30/1/1:   HMX/RDX/TNT/wax/trylene ($C_{1.986}H_{2.7825}N_{2.233}O_{2.6293}$)
16. EDC-24: 95/5 HMX/wax ($C_{5.113}H_{10.252}N_8O_8$)
17. EDNA: ethylene dinitramine ($C_2H_6N_4O_4$)
18. Ethriol trinitrate: $C_6H_{11}N_3O_9$
19. Explosive D: ammonium picrate ($C_6H_6N_4O_7$)
20. HBX-1: $C_{2.068}H_{2.83}N_{1.586}O_{2.085}Al_{0.63}$
21. HMX: cyclotetramethylenetetranitramine ($C_4H_8N_8O_8$)
22. HMX/Al (90/10): $C_{1.216}H_{2.432}N_{2.432}O_{2.432}Al_{0.371}$
23. HMX/Al (60/40): $C_{0.812}H_{1.624}N_{1.624}O_{1.624}Al_{1.483}$
24. 75/25 HMX/hydrazine nitrate: $C_4H_{13.192}N_{11.115}O_{11.115}$
25. 6.435/2.2275/6.434 $HNO_3/H_2O/CH_3NO_2$ ($C_{6.434}H_{30.192}N_{12.869}O_{34.405}$)
26. HNS: 2,2',4,4',6,6'-hexanitrostilbene ($C_{14}H_6N_6O_{12}$)
27. LX-14: 95/5 HMX/estane ($C_{4.800}H_{9.1365}N_{8.024}O_{8.2811}$)
28. MHN: mannitol hexanitrate ($C_6H_8N_6O_{18}$)
29. NG: nitroglycerine ($C_3H_5N_3O_9$)
30. Nitromethane: CH_3NO_2
31. 1/0.071 moles   nitromethane/tetranitromethane: $C_{1.071}H_3N_{1.284}O_{2.568}$
32. 1/0.25 moles nitromethane/tetranitromethane: $C_{1.125}H_3N_2O_4$
33. 1/0.50 moles nitromethane/tetranitromethane: $C_{1.5}H_3N_3O_6$
34. Nitrourea: $CH_3N_3O_3$
35. NONA: 2,2',2'',4,4',4'',6,6',6''-nonanitrophenyl ($C_{18}H_5N_9O_{18}$)
36. OCTOL-76/23: 76.3/23.7 HMX/TNT ($C_{1.76}H_{2.58}N_{2.37}O_{2.69}$)
37. ONT: 2,2',2'',4,4',4'',6,6',6''-octanitroterphenyl ($C_{18}H_6N_8O_{16}$)
38. PBX-9011: 90/10 HMX/estane ($C_{5.696}H_{10.476}N_{8.062}O_{8.589}$)
39. PBX-9501:   95/2.5/2.5   HMX/estane/BDNPF ($C_{4.575}H_{8.8678}N_{8.112}O_{8.390}$)
40. PBXC-116: 86/14 RDX/Binder ($C_{1.968}H_{3.7468}N_{2.356}O_{2.4744}$)
41. PBXC-119: 82/18 HMX/Binder ($C_{1.817}H_{4.1073}N_{2.2149}O_{2.6880}$)
42. Pentolite: 50/50 TNT/PETN ($C_{2.332}H_{2.3659}N_{1.293}O_{3.2187}$)
43. PETN: pentaerythritol tetranitrate ($C_5H_8N_4O_{12}$)
44. PETRIN: pentaerythritol trinitrate ($C_5H_9N_3O_{10}$)
45. 95/5 PYX/polyethylene: $C_{19.33}H_{11.663}N_{11}O_{16}$
46. RDX: cyclomethylene trinitramine ($C_3H_6N_6O_6$)
47. RDX/Al (90/10): $C_{1.215}H_{2.43}N_{2.43}O_{2.43}Al_{0.371}$
48. RDX/Al (60/40): $C_{0.81}H_{1.62}N_{1.62}O_{1.62}Al_{1.483}$
49. Z-TACOT: 1,3,7,9-tetranitro-benzotriazolo-[2,1-a]benzotriazole ($C_{12}H_4N_8O_8$)
50. TATB: 1,3,5-triamino-2,4,6-trinitrobenzene ($C_6H_6N_6O_6$)
51. TETRYL: N-methyl-N-nitro-2,4,6-trinitroaniline ($C_7H_5N_5O_8$)
52. TNETB/Al (90/10): $C_{1.399}H_{1.399}N_{1.399}O_{3.264}Al_{0.371}$
53. TNETB/Al (70/30): $C_{1.088}H_{1.088}N_{1.088}O_{2.539}Al_{1.11}$
54. TNM: tetranitromethane (CN_4O_8)
55. TNT: 2,4,6-trinitrotoluene ($C_7H_5N_3O_6$)
56. TNT/Al (78.3/21.7): $C_{2.414}H_{1.724}N_{1.034}O_{2.069}Al_{0.804}$
57. 14.5/85.5 toluene/nitromethane: $C_{2.503}H_{5.461}N_{1.4006}O_{2.8013}$

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