A new approach to predict the strength of high energy materials

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ABSTRACT

This paper presents a new approach to predict the strength of energetic compounds in which there are important classes of high explosives including nitroaromatics, acyclic and cyclic nitramines, nitrate esters and nitroaliphatics. For $C_aH_bN_cO_d$ compounds, the ratio of carbon to oxygen atoms and the predicted heat of detonation on the basis of the H_2O–CO_2 arbitrary have been used to calculate the strength of an explosive. The new model can give good predictions for mentioned energetic compounds as determined by the Trauzl test. The novel correlation will be useful in predicting the strength or power of a new energetic compound that has significant potential in the field of explosives and propellants.

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1. Introduction

Heat of detonation, detonation velocity and the Chapman–Jouguet pressure are convenient parameters for describing the performance potential of an explosive [1–4]. They can be predicted by different complex and simple computer codes [5–8] or simple empirical methods [2,3]. For detonation of an explosive in a borehole, the relevant parameter is its strength. The Trauzl lead block test [9] can be used to estimate and compare the capacity of explosives for doing useful work. It is a suitable method for assessing the energy released by detonating energetic compounds [10]. For many years, this test and ballistic mortar are recognized to be suitable experimental methods for measuring the strength of explosives [11]. This test consists of a standard cast cylindrical lead block (0.200 m height and 0.200 m diameter), which has an axial recess of 0.025 m diameter and 0.125 m depth. The lead block is charged with 10 g sample and detonator that is stemmed with quartz sand. The shot is fired and the volume expansion of the cavity is recorded.

While the Trauzl lead block test itself is extremely easy to implement, the results are not often reproducible, and is very sensitive to impurity and composition of explosive. For example, reported volume expansion values of cyclo-1,3,5-trimethylene-2,4,6-trinitramine (RDX) vary from 465 to 520 × 10^6 m^3 [12]. Trauzl test is considered to provide only a crude, qualitative estimate of an explosive's power, and its results are often considered to be suspect. For evaluation of high explosives in the Trauzl test, conical fractures along the periphery of the base of the block were observed, which can be related to shock energy [13]. For CHNO-type explosives, strength is dependent to a large extent on the volume of gases and the heat produced upon detonation explosive [14]. Different methods have been developed to estimate an explosive strength, which were used for commercial explosives in Russian country [12,15,16]. Explosion heat and volume of explosions are two variables that have been employed in all of them. Kuznetsov and Shatsukevich [12] introduced the relative efficiency of an explosion (A_{rel}) as a new quantity rather than conventional relative strength (f) to obtain volume expansion. Afanasenkov et al. [15] have tried to obtain a formula for the relative strength of commercial explosives. They have determined the strength for mixtures of Amatol (79/21 AN/TNT) with various additives as well as mixtures of ammonium nitrate and aluminum of various compositions. Later, Afanasenkov [16] has stated that assumptions of Kuznetsov and Shatsukevich [12] are not correct for predicting the values of volume expansion. Another correlation was introduced by Afanasenkov [16] to predict volume expansion in the Trauzl lead block on the basis of reported values of explosion heat and volume of explosion products.

In this paper, we will introduce a reliable simple correlation for predicting the strength of nitroaromatics, acyclic and cyclic nitramines, nitrate esters and nitroaliphatics considered as some important classes of energetic compounds. It will be shown that the heat of detonation on the basis of the H_2O–CO_2 arbitrary and the ratio of carbon to oxygen can be used to derive a novel correlation. In contrast to previous works [12,16] that are complex to use, the new correlation depends on only simple parameters that provide good results by calculation. The method will be applied to both
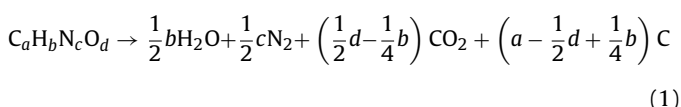
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pure explosives and explosive formulations, and compared against experimental values, where known.

2. Important parameters for predicting the power of energetic compounds

The strength of high explosives can be correlated with detonation performance through the heat of detonation and volume of gaseous detonation products. The heat of detonation is the energy available to do mechanical work and potential damage to surroundings [17,18]. It is a quantity used to assess a candidate's detonation performance that can be determined from the heats of formation of the reactants and the products of the detonation. For an explosive having the general formula $C_aH_bN_cO_d$, Kamlet and Jacobs [19] have suggested that if there is at least enough oxygen to convert hydrogen to H_2O but no more than is also required to convert carbon to CO_2, the product compositions can be represented by the "H_2O–CO_2 arbitrary". The decomposition predicts N_2, H_2O and CO_2 as the important detonation products:

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

$$(1)$$

According to Eq. (1), the heat of detonation can be determined from the heats of formation of the reactants and detonation products of the detonation through the following relation:

$$Q_{H_2O-CO_2}$$

$$= \frac{-\frac{b}{2}\Delta_f H^\theta(H_2O) - \left(\frac{1}{2}d - \frac{1}{4}b\right)\Delta_f H^\theta(CO_2) + \Delta_f H^\theta(\text{explosive})}{\text{formula weight of explosive}}$$

$$(2)$$

If the composition and the heat of formation of an explosive were known, Eq. (2) can provide a simple way to calculate the heat of detonation. Fortunately, simple empirical and quantum mechanical methods have been recently developed to find the condensed

Fig. 1. Calculated the expansion in the Trauzl lead block versus experimental values for 39 energetic compounds.

phase heat of formation of different classes $C_aH_bN_cO_d$ energetic compounds [20–23], which can be used in Eq. (2). The calculated values of $Q_{H_2O-CO_2}$ for some energetic compounds including nitroaromatics, acyclic and cyclic nitramines, nitrate esters and nitroaliphatics are given in Table 1. For the predicted heats of detonation, H_2O is assumed to be in the liquid state. The experimental values of the expansion in the Trauzl lead block of these compounds (ΔV_{Trauzl}) have also been given in Table 1.

The number of moles of gaseous detonation products may be another important factor that can be used to derive a suitable correlation. In addition to appropriate decomposition reactions such as Eq. (1), determination of the equilibrium composition of the product gases can also be made through experimental measurement and thermochemical equilibrium calculations. For example, the study of the product concentrations predicted by the Cheetah 2.0/JCZS calculations was indicated for 34 $C_aH_bN_cO_d$ explosives that 94% of the gaseous products consist of H_2O, H_2, N_2, CO and CO_2 [18]. However, the following equation shows the various detonation products that can be specified by a suitable thermochemical codes such as Cheetah 2.0/JCZS:

$$C_aH_bN_cO_d \rightarrow eH_2O + fN_2 + gCO_2 + hCO + iH_2 + jC$$

$$+ k(\text{other products}) \qquad (3)$$
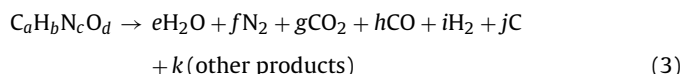
3. Results and discussion

The study of various situations has shown that suitable combination of elemental composition can be used to introduce the effect of the number of moles of gaseous products on ΔV_{Trauzl} in addition to $Q_{H_2O-CO_2}$. For $C_aH_bN_cO_d$ nitroaromatics, it was found that the ratios of the number of carbon to oxygen ($r_{a/d}$) and hydrogen to oxygen ($r_{b/d}$) atoms are important factors for correcting the predicted heats of detonation by the H_2O–CO_2 arbitrary with respect to experimental data [24]. The values of $r_{a/d}$ and $r_{b/d}$ can also affect the equilibrium composition of different decomposition products in Eq. (3). Of two mentioned ratios, the ratio $r_{a/d}$ has appreciable effect in improving the predicted ΔV_{Trauzl} on the basis $Q_{H_2O-CO_2}$. Meanwhile, the effect of $r_{b/d}$ on ΔV_{Trauzl} is negligible that can be omitted. To find the relationship between two parameters of $r_{a/d}$ and $Q_{H_2O-CO_2}$ with ΔV_{Trauzl}, various combinations of $r_{a/d}$ and $Q_{H_2O-CO_2}$ have been examined and optimized with experimental data given in Table 1. The optimized correlation has the following form:

$$\Delta V_{\text{Trauzl}} = -135.35 \times 10^{-6} r_{a/d} + 77.39 \times 10^{-6} Q_{H_2O-CO_2} \qquad (4)$$

Although uncertainty in determination of ΔV_{Trauzl} is relatively high, the coefficient of determination (R^2) of Eq. (4) is relatively good that is equal to 0.90 [25]. There are 53 measured values (corresponding to 39 molecules) for ΔV_{Trauzl} values in Table 1. Predicted values of ΔV_{Trauzl} using Eq. (4) are also given in Table 1. Fig. 1 shows the effect of inclusion of parameter $r_{a/d}$ in Eq. (4) for improvement of the predicted results on the basis $Q_{H_2O-CO_2}$. In Fig. 1, the solid line shows exact agreement between predictions and experiment. The root mean square (rms) deviation of new correlation from experiment is 11.2%. Since the value of ΔV_{Trauzl} potentially embeds significant errors, Eq. (4) can also be represented as the relative strength in form $f = \Delta V_{\text{Trauzl}}/\Delta V_{\text{Trauzl}}$ (standard). The quantity f could be a relevant and useful parameter for qualitatively characterizing the strength of an explosive if the error associated with it remains less than the error associated with ΔV_{Trauzl}. The relative strength f has been widely used for quantitative comparison the action of explosions of different high explosives [15,16]. Different suitable energetic compounds such as TNT and Amatol can be used as the standard high explosives. The relative strengths for different
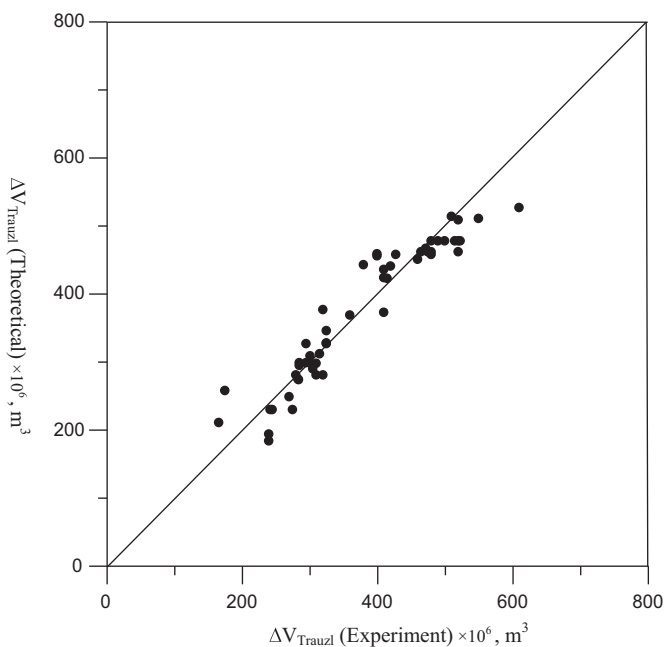
Table 1
Comparison of the predicted ΔV_{Trauzl} and the relative strength from the present new method with experimental data.

Compound	Molecular Formula	$Q_{H_2O-CO_2}$ (kJ/g)	Strength experiment $\times 10^6$ (m³)	Strength new method $\times 10^6$ (m³)	%Dev$_1$[a]	f_{exp}	f_{cal}	%Dev$_2$[b]
1,3-Bis(2,2,2-trinitroethyl)urea (BTNEU)	$C_5H_6N_8O_{13}$	6.486	460 [27]	450	2.2	1.56	1.53	3.4
1,3,5,7-Tetranitro-1,3,5,7-tetrazocane (HMX)	$C_4H_8N_8O_8$	6.777	480 [9]	457	4.8	1.63	1.55	7.8
			428 [28]		−6.8	1.45		−9.9
1,3,5-Trinitro-1,3,5-triazinane (RDX)	$C_3H_6N_6O_6$	6.825	480 [9]	461	4.0	1.63	1.56	6.4
			465 [12]		0.9	1.58		1.4
			475 [12]		2.9	1.61		4.7
			520 [12]		11.3	1.76		20.0
{2-[2-(Nitrooxy)ethoxy]ethyl} nitrate	$C_4H_8N_2O_7$	6.618	410 [9]	435	−6.1	1.39	1.47	−8.5
(2-{Nitro[2-(nitrooxy)ethyl]amino}ethyl) nitrate (DINA)	$C_4H_8N_4O_8$	6.896	472 [29]	466	1.3	1.60	1.58	2.0
{3-[3-(Nitrooxy)-2,2-bis[(nitrooxy)methyl]propoxy]-2,2-bis[(nitrooxy)methyl]propyl} nitrate (DPEHN)	$C_{10}H_{16}N_6O_{19}$	6.629	380 [30]	442	−16.3	1.29	1.50	−21.0
[1,3,4-Tris(nitrooxy)butan-2-yl] nitrate	$C_4H_6N_4O_{12}$	7.170	550 [27]	510	7.3	1.86	1.73	13.6
2,2-Bis(nitrooxymethyl)butyl nitrate	$C_6H_{11}N_3O_9$	6.621	415 [9]	422	−1.7	1.41	1.43	−2.4
Nitro[2-(nitroamino)ethyl]amine (EDNA)	$C_2H_6N_4O_4$	6.339	410 [9]	423	−3.2	1.39	1.43	−4.4
Ethyl nitrate	$C_2H_5NO_3$	6.845	420 [9]	440	−4.8	1.42	1.49	−6.8
1,3,4,5,6-Pentakis(nitrooxy)hexan-2-yl nitrate (*MHN*)	$C_6H_8N_6O_{18}$	7.217	510 [9]	513	−0.6	1.73	1.74	−1.0
Methyl nitrate	CH_3NO_3	7.381	610 [9]	526	13.8	2.07	1.78	28.5
1-(Nitrooxy)-2,2-bis[(nitrooxy)methyl]propane	$C_5H_9N_3O_9$	6.852	400 [9]	455	−13.8	1.36	1.54	−18.6
[1,3-Bis(nitrooxy)propan-2-yl] nitrate	$C_3H_5N_3O_9$	7.149	520 [9]	508	2.3	1.76	1.72	4.1
1-Nitroguanidine	$CH_4N_4O_2$	4.606	305 [9]	289	5.2	1.03	0.98	5.4
Nitromethane	CH_3NO_2	6.792	400 [9]	458	−14.5	1.36	1.55	−19.7
Nitrourea	$CH_3N_3O_3$	4.207	310 [9]	280	9.7	1.05	0.95	10.2
			320 [9]		12.5	1.08		13.6
[3-(Nitrooxy)-2,2-bis[(nitrooxy)methyl]propyl] nitrate (PETN)	$C_5H_8N_4O_{12}$	6.895	523 [9]	477	8.8	1.77	1.62	15.6
			480 [31]		0.6	1.63		1.0
			490 [31]		2.7	1.66		4.4
			500 [31]		4.6	1.69		7.8
			515 [31]		7.4	1.75		12.9
			520 [31]		8.3	1.76		14.6
(2-{2-[2-(Nitrooxy)ethoxy]ethoxy}ethyl) nitrate (TEGN)	$C_6H_{12}N_2O_8$	6.168	320 [9]	376	−17.5	1.08	1.27	−19.0
Oxoazinic acid, urea	$CH_5N_3O_4$	3.637	270 [9]	248	8.1	0.92	0.84	7.5
Ammonium 2,4,6-trinitrobenzen-1-olate	$C_6H_6N_4O_7$	5.115	280 [9]	280	0.0	0.95	0.95	0.0
1-Methyl-2,4-dinitro benzene	$C_7H_6N_2O_4$	5.420	240 [9]	183	23.8	0.81	0.62	19.3
2-Methyl-1,3-dinitrobenzene	$C_7H_6N_2O_4$	5.554	240 [9]	193	19.6	0.81	0.65	15.9
N-Ethyl-N,2,4,6-tetranitroaniline	$C_8H_7N_5O_8$	6.207	325 [9]	345	−6.2	1.10	1.17	−6.8
2,4,6-Trinitro-N-(2,4,6-trinitrophenyl)aniline	$C_{12}H_5N_7O_{12}$	5.980	325 [9]	327	−0.6	1.10	1.11	−0.7
1,3,5-Trinitro-2-[(E)-2-(2,4,6-trinitrophenyl)ethenyl]-Benzene	$C_{14}H_6N_6O_{12}$	6.015	301 [9]	308	−2.3	1.02	1.04	−2.4
1,3-Dinitrobenzene	$C_6H_4N_2O_4$	5.585	242 [9]	229	5.4	0.82	0.78	4.4
			245 [30]		6.5	0.83		5.4
			275 [30]		16.7	0.93		15.6
2-Amino-4,6-dinitrophenol	$C_6H_5N_3O_5$	4.816	166 [9]	210	−26.5	0.56	0.71	−14.9
2,4,6-Trinitrophenol	$C_6H_3N_3O_7$	5.513	315 [9]	311	1.3	1.07	1.05	1.4
2,4,6-Trinitrobenzene-1,3-diol (TNR)	$C_6H_3N_3O_8$	4.835	284 [9]	273	3.9	0.96	0.92	3.7
N-methyl-N,2,4,6-tetranitroaniline (Tetryl)	$C_7H_5N_5O_8$	6.331	410 [9]	372	9.3	1.39	1.26	12.9
2-Methyl-1,3,5-trinitrobenzene (TNT)	$C_7H_5N_3O_6$	5.888	300 [9]	298	0.7	1.02	1.01	0.7
			285 [32]		−4.6	0.97		−4.4
			295 [32]		−1.0	1.00		−1.0
2,4,6-Trinitrobenzene-1,3,5-triamine (TATB)	$C_6H_6N_6O_6$	5.071	175 [9]	257	−46.9	0.59	0.87	−27.8
2,4,6-Trinitroaniline (TNA)	$C_6H_4N_4O_6$	5.592	310 [9]	297	4.2	1.05	1.01	4.4
2-Methoxy-1,3,5-trinitrobenzene	$C_7H_5N_3O_7$	5.955	295 [9]	326	−10.5	1.00	1.10	−10.5
1,3,5-Trinitrobenzene	$C_6H_3N_3O_6$	5.966	325 [9]	326	−0.3	1.10	1.11	−0.3
2,4,6-Trinitrobenzoic acid	$C_7H_3N_3O_8$	5.076	283 [9]	274	3.2	0.96	0.93	3.1
3-Methyl-2,4,6-trinitrophenol	$C_7H_5N_3O_7$	5.547	285 [9]	294	−3.2	0.97	1.00	−3.1
[2-Hydroxy-2-(2,4,6-trinitrophenyl)ethyl] nitrate	$C_8H_6N_4O_{10}$	6.156	356 [31]	368	−2.3	1.22	1.25	−2.7
rms deviation (%)					11.2			11.3

[a] $\%\text{Dev}_1 = \frac{\text{Strength experiment} - \text{Strength new method}}{\text{Strength experiment}} \times 100$.

[b] $\%\text{Dev}_2 = (f_{\text{exp}} - f_{\text{cal}}) \times 100$.

Table 2
Comparison of the predicted ΔV_{Trauzl} and the relative strength from the present new method with experimental data for some energetic compounds that have complex molecular structures.

Compound	Molecular formula	$Q_{H_2O-CO_2}$ (kJ/g)	Strength experiment $\times 10^6$ (m^3)	Strength new method $\times 10^6$ (m^3)	%Dev$_1$ [a]	f_{exp}	f_{cal}	%Dev$_2$ [b]
6-Diazo-2,4-dinitro-2,4-cyclohexadien-1-one	$C_6H_2N_4O_5$	6.145	326 [9]	313	4.0	1.11	1.06	4.4
1,3,5-Triazido-2,4,6-trinitrobenzene	$C_6N_{12}O_6$	6.875	470 [9]	397	15.5	1.59	1.34	24.7
2-(2,4,6-Trinitrophenoxy)-ethanol nitrate	$C_8H_6N_4O_{10}$	6.156	350 [9]	368	−5.1	1.19	1.25	−6.1
3-Methyl-1,2,4,5-tetranitrobenzene	$C_7H_4N_4O_8$	6.884	398 [29]	414	−4.0	1.35	1.40	−5.3
2,4-Dinitrophenol	$C_6H_4N_2O_5$	6.115	243 [9]	311	−28.0	0.82	1.05	−23.1
Ammonium nitrate (AN)	$H_4N_2O_3$	2.656	180 [9]	206	−14.4			−8.8
2-(Dinitromethylidene)imidazolidine-4,5-diol	$C_4H_6N_4O_6$	5.649	360 [9]	347	3.6	1.22	1.18	4.4
2-Aminoethyl nitrate; nitric acid	$C_2H_7N_3O_6$	6.185	410 [9]	434	−5.9	1.39	1.47	−8.1
Ethane-1,2-diamine; nitric acid	$C_2H_{10}N_4O_6$	4.858	350 [9]	331	5.4	1.19	1.12	6.4
Guanidine; nitric acid	$CH_4N_4O_3$	4.015	240 [9]	266	−10.8	0.81	0.90	−8.8
Hydrazine nitrate	$H_5N_3O_3$	5.072	408 [9]	393	3.7	1.38	1.33	5.1
Methanamine, nitric acid	$CH_6N_2O_3$	5.375	325 [9]	371	−14.2	1.10	1.26	−15.6
[2-Nitro-3-(nitrooxy)-2-[(nitrooxy)methyl]propyl]-nitrate (NIBTN)	$C_4H_6N_4O_{11}$	7.704	540 [9]	547	−1.3	1.83	1.85	−2.4
Methyl nitrate	CH_3NO_3	7.381	600 [9]	526	12.3	2.03	1.78	25.1
Ethyl nitrate	$C_2H_5NO_3$	6.847	422 [9]	440	−4.3	1.43	1.49	−6.1
1,3-Dinitroimidazolidin-2-one	$C_3H_4N_4O_5$	5.861	354 [33]	372	−5.1	1.20	1.26	−6.1
{1,3,3-Tris[(nitrooxy)methyl]-2-oxocyclopentyl}-methyl nitrate	$C_9H_{12}N_4O_{13}$	6.294	380 [33]	393	−3.3	1.29	1.33	−4.2
N-(nitramidomethyl)nitramide (MEDINA)	$CH_4N_4O_4$	6.673	437 [31]	483	−10.6	1.48	1.64	−15.7
nitro[2-(nitroamino)ethyl]amine (EDNA)	$C_2H_6N_4O_4$	6.339	360 [27]	423	−17.5	1.22	1.43	−21.4
Dinitroethane	$C_2H_4N_2O_4$	6.557	443 [29]	440	0.6	1.50	1.49	0.8
Dinitropropane	$C_3H_6N_2O_4$	6.326	383 [29]	388	−1.2	1.30	1.32	−1.5
2,2-Dinitropropane-1,3-diol	$C_3H_6N_2O_6$	6.935	540 [31]	469	13.1	1.83	1.59	24.1
2-(Nitrooxy)ethane-1-ol	$C_2H_5NO_4$	5.919	375 [33]	390	−4.0	1.27	1.32	−5.1
2,2,5,5-Tetramethylolcyclopentanol pentanitrate (FIVOLITE)	$C_9H_{13}N_5O_{15}$	6.792	472 [33]	444	5.9	1.60	1.51	9.5
[1,4-Di(phenyl)-1,2,4-triazol-4-ium-3-yl]- Phenylazanide (13.4% N)	$C_6H_7N2.5O_{10}$	5.355	373 [9]	333	10.7	1.26	1.13	13.6
rms deviation (%)					10.3			12.8

[a] $\%Dev_1 = \frac{\text{Strength experiment} - \text{Strength new method}}{\text{Strength experiment}} \times 100$.

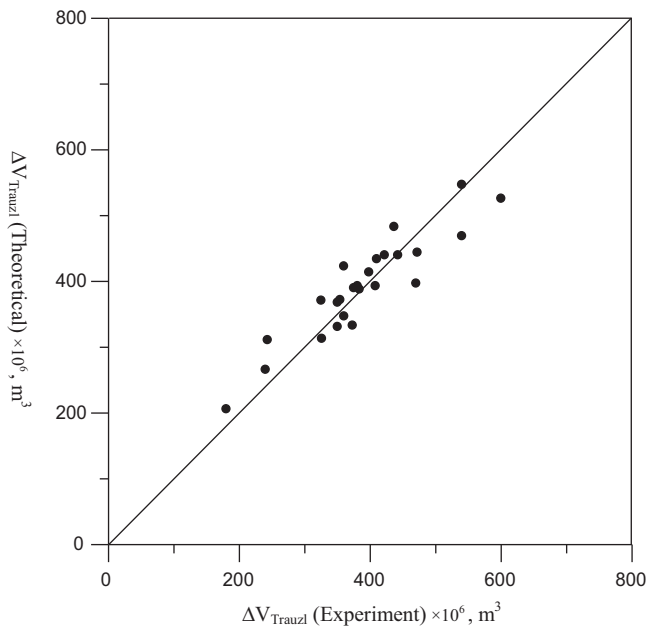[b] $\%Dev_2 = (f_{exp} - f_{cal}) \times 100$.

Fig. 2. Calculated the expansion in the Trauzl lead block versus measured values for 25 energetic compounds that have complex molecular structures.

energetic compounds using Eq. (4), f_{cal}, and corresponding experimental data, f_{exp}, have also been given in Table 1. However, there is fairly good agreement between f_{cal} and f_{exp}. It was assumed that the expansion in Trauzl lead block for TNT as the standard high explosive is equal to 295×10^{-6} m^3 (corresponding to the average value of its data given in Table 1). As seen in Table 1, the maximum deviation of ΔV_{Trauzl} from experiment is 46.9% that could be also given in terms of relative strength with respect to TNT about as 28–29%.

To estimate an average uncertainty of Trauzl lead block test, the 95% confidence limits for some CHNO explosives with several measurements given in Table 1 are on average within about $\pm 29.2\%$. The results of lead block test depend on the loading density of the explosives, the fitness of the sand used in taming, the temperature of molten lead at the time of casting and the temperature of block, which can provide the error in measurements [26].

Since Eq. (4) is introduced to aid in the calculation of the power of energetic materials that have not yet been synthesized, it is crucial that its predictive capability is assessed. To show the reliability of the novel method for energetic compounds with complex molecular structures, the calculated values of ΔV_{Trauzl} for some different $C_a H_b N_c O_d$ energetic compounds have been given in Table 2. As seen, the rms and maximum deviations of predicted ΔV_{Trauzl} from experiment are 10.3% and 28.0%, respectively. Fig. 2 provides a visual comparison between experimental and calculated values for energetic compounds given in Table 2. In Fig. 2, the points are distributed approximately equally on either side of this line.

To demonstrate the new method and test its validity for explosive formulations, the calculated values of ΔV_{Trauzl} for 11 explosive formulations are given in Table 3. Eq. (2) for predicting $Q_{H_2O-CO_2}$ is appealing because it requires only the heat of formation of the explosive and it can be applied to explosive mixtures. For an explosive formulation, the heat of formation of the mixture can be calculated from the heats of formation of the individual components [13]. As seen in Table 3, the predicted results are in good agreement with the measured values. The rms and maximum deviations of the predicted ΔV_{Trauzl} from experiment are 8.1% and 17.3%, respectively. A visual comparison of the predictions with the measured values is also given in Fig. 3. As seen in Tables 2 and 3, there is also good agreement between f_{cal} and f_{exp}.

Table 3
Comparison of the predicted ΔV_{Trauzl} and the relative strength from the present new method with experimental data for some explosive mixtures.

Compound	Molecular formula	$Q_{H_2O-CO_2}$ (kJ/g)	Strength experiment $\times 10^6$ (m^3)	Strength new method $\times 10^6$ (m^3)	%Dev$_1$[a]	f_{exp}	f_{cal}	%Dev$_2$[b]
30/70 TNT/RDX (Bonit No. 2)	C$_{1.871}$H$_{2.553}$N$_{2.288}$O$_{2.685}$	6.55	421 [29]	413	1.9	1.43	1.40	2.7
60/40 TNT/Hexanitrodiphenylamine (Novit 60/40)	C$_{2.944}$H$_{1.777}$N$_{1.431}$O$_{2.679}$	5.935	310 [29]	311	−0.4	1.05	1.05	−0.4
60/50 TNT/Hexanitrodiphenylamine (Novit 50/50)	C$_{2.909}$H$_{1.671}$N$_{1.458}$O$_{2.688}$	5.943	315 [31]	313	0.6	1.07	1.06	0.7
50/50 TNT/PETN (PENTOLITE)	C$_{2.333}$H$_{2.367}$N$_{1.294}$O$_{3.220}$	6.4	359.9 [31]	397	−10.3	1.22	1.35	−12.6
80/20 AN/TNT	C$_{0.617}$H$_{4.441}$N$_{2.264}$O$_{3.529}$	5.272	430 [34]	384	10.7	1.46	1.30	15.6
70/30 AN/RDX	C$_{0.405}$H$_{4.311}$N$_{2.561}$O$_{3.436}$	5.627	450 [34]	419	6.9	1.53	1.42	10.5
70/30 AN/PETN	C$_{0.475}$H$_{4.259}$N$_{2.130}$O$_{3.764}$	5.646	450 [34]	420	6.7	1.53	1.42	10.2
60/40 TNT/RDX	C$_{2.391}$H$_{2.403}$N$_{1.874}$O$_{2.667}$	6.274	440 [34]	364	17.3	1.49	1.23	25.8
80/20 PETN/NG	C$_{1.530}$H$_{2.4666}$N$_{1.277}$O$_{3.831}$	6.946	530 [33]	483	8.9	1.80	1.64	15.9
70/30 PETN/NG	C$_{1.504}$H$_{2.433}$N$_{1.283}$O$_{3.848}$	6.971	510 [33]	487	4.5	1.73	1.65	7.8
92/8 NG/NC (Blasting gelatin)	C$_{1.399}$H$_{2.240}$N$_{1.284}$O$_{3.937}$	6.55	421 [29]	413	1.9	1.43	1.40	2.7
rms deviation (%)					8.1			12.1

[a] %Dev$_1$ = $\frac{\text{Strength experiment} - \text{Strength new method}}{\text{Strength experiment}} \times 100$.

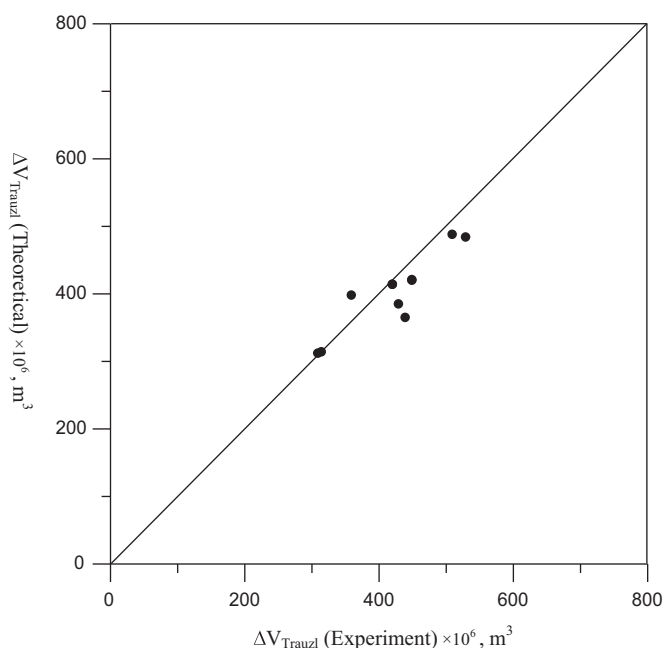[b] %Dev$_2$ = $(f_{exp} - f_{cal}) \times 100$.

Fig. 3. Calculated the expansion in the Trauzl lead block versus experimental values for 11 explosive formulations.

Explosive nitrate salts can be classified as nonideal explosives. Nonideal explosives have significantly different detonation properties than predicted by equilibrium and physical separation of the fuel and oxidizer in such explosive result in extended chemical reaction zones. Since nitrate salts exhibits nonideal detonation behavior, the amount of reacted material may be function of the reaction zone length. As indicated in Tables 1 and 2, the new correlation can be easily applied to some energetic salts such as urea nitrate and ammonium nitrate, which have nonideal behavior.

Cage explosives have favorable properties such as high density that can provide high performance. The new model can also be used for this category of energetic materials. For example, CL-20 [2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNIW)] is a new high performance nitramine explosive, which has $Q_{H_2O-CO_2} = 6.864$ kJ/g. The predicted ΔV_{Trauzl} of this compound by new method is 464×10^{-6} m^3 that is consistent with the experimental values of HMX and RDX given in Table 1.

According to the predicted results, the new model has some advantages with respect to the other methodologies:

1. The correlation coefficient of Eq. (4) is relatively good with respect to large uncertainty in experimental data of Table 1, e.g. two different values of ΔV_{Trauzl} (480×10^{-6} and 428×10^{-6} m^3) were reported for HMX. As seen in Table 2, Eq. (4) provides good results for energetic compounds with complex molecular structures, which confirms the reliability of new correlation for wide range classes of energetic compounds. Meanwhile, previous works were tested only for commercial explosives in which well-known explosives were used.
2. Two variables $r_{a/d}$ and $Q_{H_2O-CO_2}$ in Eq. (4) can be easily calculated for any pure and mixture of CHNO energetic compounds.

4. Conclusions

A novel simple method has been introduced, which uses only the ratio of carbon to oxygen and the calculated $Q_{H_2O-CO_2}$ to predict the strength of different classes of $C_aH_bN_cO_d$ energetic compounds. In this method, the detonation products are assumed to correspond to the H_2O-CO_2 arbitrary, in which the products are limited to N_2, H_2O, CO_2 and solid carbon. The new method can be used easily to any $C_aH_bN_cO_d$ material without any need to use computer codes. As indicated in Tables 1–3, Eq. (4) provides reliable results with respect to experiment for pure explosives and explosive mixtures.

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