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New method for calculating densities of nitroaromatic explosive compounds

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Abstract

A new model has been introduced for simple calculation of crystal density of an important class of organic explosives, namely nitroaromatic energetic compounds. This model is based on the fundamental correlation. The introduced procedure has been applied to 60 well-known and new synthesized organic nitroaromatic explosives. The results show that the present method gives comparable prediction respect to well-developed group additivity method for estimation of crystal density of organic explosives. The introduced simple method can be applied to any complex nitroaromatic explosive that contains the elements of carbon, hydrogen, nitrogen and oxygen with no difficulties.
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1. Introduction

Simple methods can facilitate the discovery of new energetic materials that have significant advantages over materials currently in use. Properties such as density, heat of formation, detonation pressure, detonation velocity and sensitivity can help us to screen potential energetic candidates would permit the selection of only the most promising substances for laboratory synthesis, scale-up, testing, etc. However, predicting crystal density is one of the most important properties of high explosives. The solid-state density is affected the amount of material that can be packed into a volume-limited warhead or propulsion configuration. For most explosives, the detonation velocity increases linearly with density while the Chapman–Jouguet pressure is proportional to the square of the loading density [1].

To a chemist concerned with the synthesis of new high explosive compounds the ability to estimate crystal density and heat of formation from a given molecular structure is a problem of the utmost importance because they are usually needed to evaluate detonation properties by a computer code or empirical methods. The calculated detonation properties could be meaningful in the decision as to whether it is worth the effort to attempt a new and complex synthesis. The major goals of thermochemical codes and empirical methods apart from being developed as predictive tools, is to provide insight to understanding the molecules which are responsible for higher performance and which are not. An equilibrium complicated thermochemical code such as TIGER [2] and equations of state for detonation products can be used to estimate detonation parameters for explosives as well as parameters for other conditions such as a constant explosion. Each equation of state has a different set of data that mirrors the preferences of the workers that use it. Some well-known equations of state are Becker–Kistiakowsky–Wilson (BKW) [3], the Jacobs–Cowperthwaite–Zwisler (JCZ) [4,5] and Kihara–Hikita–Tanaka (KHT) [6]. New empirical methods were recently introduced for reliable detonation and thermochemical properties of ideal and non-ideal pure or mixed explosives of different classes [7–18].

Density and heat of formation usually are two parameters which are necessary in evaluating the performance of explosives by computer codes and empirical methods. Studies show that detonation velocity and pressure are greatly sensitive to density values, but somewhat less sensitive to the heat of formation [10,13,14]. Therefore, predicting the crystal density of unsynthesized organic explosives is one of the important data to explosive user for determining the performance of explosives. Molecular structure of an explosive can be related to its density [19]. Theoretical and empirical nature methods are two broad

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categories to estimate the density of compounds. Some studies have been attempting to predict crystal densities based on the arrays of 3D molecular by using computational chemistry, but this prediction is still a formidable task and is known to have several huge hurdles in getting the job in a right fashion so that only some applications have been found in the area of energetic materials [20–24]. Additive constituent volumes were used by the empirical methods for estimating the molar volume, which are simple and relatively accurate [25–29]. Of different methods of estimating density of energetic materials, many researchers tend to utilize the empirical methods. Empirical methods based on summing up the volume of each atom or molecular fragment, such as Tarver method [28], have some restrictions that cannot be applied to some organic high explosives, e.g. some new synthesized nitroaromatic high explosives. The purpose of this work is to present a new approach for obtaining crystal density of organic high explosives. The introduced model can provide the simplest procedure for calculating density of any complex $C_a H_b N_c O_d$ molecular structure nitroaromatic high explosives only from the explosive's elemental composition. However, the main intent was to investigate the likelihood of obtaining a simple scheme for calculating the crystal density of an important class of explosives, namely nirtoaromatic high explosives, as one of the explosive parameters of somewhat more practical importance to the explosive user. The method has been tested on well-known and some new synthesized explosives, where exper-

imental data are available, and compared with Tarver method [28] where calculation is possible by this method. It should be noted that the results predicted by this simple method are comparable with the other complicated procedures which indicate the accuracy is not necessarily enhanced by greater complexity.

2. New approach for determining crystal density of nitroaromatic explosives

Since greater relevance for synthesis, performance and vulnerability predictions, the importance of a prediction tool is also increases. One of the major challenges to chemical industry is to find new explosives with a given performance, sensitivity and physical properties. Modifying known substances with higher densities such as by addition and modification of energetic groups in the molecules are usually used in practice to design new energetic compounds. Scientists tend to synthesize new generations of more powerful energetic compounds with improved properties such as high detonation velocity, reduced vulnerability, low shock and sensitivity over those in current use.

As a first attempt to express crystal density of $C_a H_b N_c O_d$ high explosives as a function of elemental composition, the results show that the following general equation with four adjustable coefficients is suitable for most nitroaromatic high explosives:

$$\rho_0 = x_1 a' + x_2 b' + x_3 c' + x_4 d' \tag{1}$$

Table 1
Density estimation for 25 well-known solid aromatic explosives by new method and Tarver method [28]

Explosive	Measured density (g/cm³)[a]	a'	b'	c'	d'	Calculated density (g/cm³) by new method[b]	% error	Calculated density (g/cm³) by Tarver method	% error
o-Dinitrobenzene	1.565	0.03571	0.02381	0.01190	0.02381	1.580 [Eq. (2)]	0.962	1.572	0.447
m-Dinitrobenzene	1.575	0.03571	0.02381	0.01190	0.02381	1.580 [Eq. (2)]	0.314	1.572	0.190
p-Dinitrobenzene	1.625	0.03571	0.02381	0.01190	0.02381	1.580 [Eq. (2)]	2.766	1.572	3.262
1,3,5-Trinitrobenzene	1.688	0.02817	0.01408	0.01408	0.02817	1.719 [Eq. (2)]	1.816	1.709	1.244
1,2,4-Trinitrobenzene	1.73	0.02817	0.01408	0.01408	0.02817	1.719 [Eq. (2)]	0.656	1.709	1.214
Hexanitrobenzene	1.988	0.01724	0.00000	0.01724	0.03448	1.919 [Eq. (2)]	3.452	1.954	1.710
3,5-Dinitrophenol	1.702	0.03261	0.02174	0.01087	0.02717	1.683 [Eq. (2f)]	1.129	1.658	2.585
2,3-Dinitrophenol	1.681	0.03261	0.02174	0.01087	0.02717	1.683 [Eq. (2f)]	0.106	1.658	1.368
2,4-Dinitrophenol	1.683	0.03261	0.02174	0.01087	0.02717	1.683 [Eq. (2f)]	0.013	1.658	1.485
3,4-Dinitrophenol	1.672	0.03261	0.02174	0.01087	0.02717	1.683 [Eq. (2f)]	0.645	1.658	0.837
Picric acid	1.763	0.02620	0.01310	0.01310	0.03057	1.788 [Eq. (2f)]	1.175	1.778	0.851
Styphnic acid	1.829	0.02449	0.01224	0.01224	0.03265	1.814 [Eq. (2f)]	0.893	1.843	0.765
2,4-Dinitrotoluene	1.521	0.03846	0.03297	0.01099	0.02198	1.518 [Eq. (2)]	0.197	1.505	1.052
2,4,6-Trinitrotoluene (TNT)	1.654	0.03084	0.02203	0.01322	0.02643	1.660 [Eq. (2)]	0.384	1.636	1.088
2,3,4-Trinitrotoluene	1.62	0.03084	0.02203	0.01322	0.02643	1.660 [Eq. (2)]	2.491	1.636	0.988
2,4,5-Trinitrotoluene	1.62	0.03084	0.02203	0.01322	0.02643	1.660 [Eq. (2)]	2.491	1.636	0.988
2,4,6-Trinitro-*m*-xylene	1.604	0.03320	0.02905	0.01245	0.02490	1.609 [Eq. (2)]	0.301	1.577	1.683
2,3,6-Trinitro-*p*-xylene	1.59	0.03320	0.02905	0.01245	0.02490	1.609 [Eq. (2)]	1.184	1.577	0.818
1,3,5-Trimethyl-2,4,6-trinitrobenzene	1.48	0.03529	0.03529	0.01176	0.02353	1.563 [Eq. (2)]	5.605	1.528	3.243
2,4-Dinitroaniline	1.615	0.03279	0.02732	0.01639	0.02186	1.617 [Eq. (2)]	0.139	1.654	2.415
2,4,6-Trinitroaniline	1.762	0.02632	0.01754	0.01754	0.02632	1.739 [Eq. (2)]	1.284	1.775	0.738
2,3,4,6-Tetranitraniline	1.867	0.02198	0.01099	0.01832	0.02930	1.821 [Eq. (2)]	2.450	1.867	0.000
1,3-Diamino-2,4,6-trinitrobenzene	1.837	0.02469	0.02058	0.02058	0.02469	1.792 [Eq. (2f)]	2.423	1.838	0.054
1,3,5-Triamino-2,4,6-trinitrobenzene	1.938	0.02326	0.02326	0.02326	0.02326	1.955 [Eq. (2e)]	0.889	1.897	2.116
3-Methyl-2,4,6-trinitrophenol	1.69	0.02817	0.01408	0.01408	0.02817	1.719 [Eq. (2)]	1.695	1.707	1.006
rms deviation							1.907		1.546

[a] Measured densities were obtained from Ref. [28].
[b] Used equations are given in bracket.

Table 2
Density estimation for some aromatic explosives where Tarver method [28] cannot be used
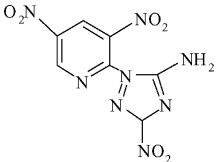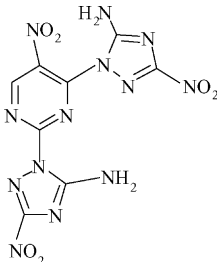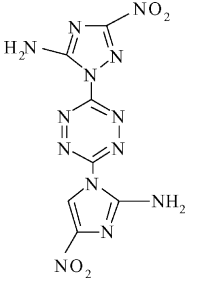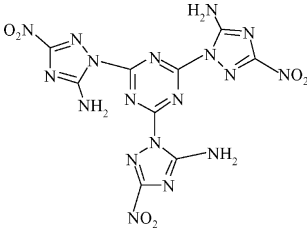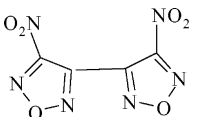
Explosive	Measured density (g/cm^3)[a]	a'	b'	c'	d'	Calculated density (g/cm^3) by new method[b]	% error
2,4,6-Trinitrocresol	1.68	0.0288	0.0206	0.0123	0.0288	1.696 [Eq. (2)]	0.942
Trinitropyridine	1.77	0.0234	0.0093	0.0187	0.0280	1.803 [Eq. (2)]	1.840
Hexanitrostilbene	1.74	0.0311	0.0133	0.0133	0.0267	1.674 [Eq. (2)]	3.794
Dinitrodiphenylamine	1.42	0.0463	0.0347	0.0116	0.0154	1.390 [Eq. (2)]	2.141
2,4,6,2′,4′,6′-Hexanitrodiphenyl amine	1.64	0.0273	0.0114	0.0159	0.0273	1.682 [Eq. (2)]	2.547
2,4,6,2′,4′,6′-Hexanitrobiphenyl	1.6	0.0283	0.0094	0.0142	0.0283	1.670 [Eq. (2g)]	4.393
Ammonium picrate	1.72	0.0244	0.0244	0.0163	0.0285	1.687 [Eq. (2d)]	1.923
Glycero-2,4-dinitrophenyl ether dinitrate	1.6	0.0259	0.0230	0.0115	0.0316	1.664 [Eq. (2d)]	3.989
Trinitrophenoxethyl nitrate	1.68	0.0252	0.0189	0.0126	0.0314	1.688 [Eq. (2d)]	0.473
Trinitroanisol	1.61	0.0288	0.0206	0.0123	0.0288	1.611 [Eq. (2d)]	0.081
Dinitrophenoxyethylnitrate	1.6	0.0293	0.0256	0.0110	0.0293	1.589 [Eq. (2d)]	0.689
2,4,6,2′,4′,6′-Hexanitrodiphenyl oxide	1.7	0.0273	0.0091	0.0136	0.0295	1.671 [Eq. (2d)]	1.713
Trinitropyridine-N-oxide	1.86	0.0217	0.0087	0.0174	0.0304	1.882 [Eq. (2c)]	1.187
Diazodinitrophenol	1.63	0.0286	0.0095	0.0190	0.0238	1.630 [Eq. (2a)]	0.018
1,3,5-Triazido-2,4,6-trinitrobenzene	1.805	0.0179	0.0000	0.0357	0.0179	1.805 [Eq. (2a)]	0.004
Benzotris(1,2,5-oxadiazole-1-oxide)	1.87	0.0238	0.0000	0.0238	0.0238	1.813 [Eq. (2)]	3.058
Tetranitrodibenzo-1,3a,4,6a-tetrazapentalene	1.85	0.0309	0.0103	0.0206	0.0206	1.850 [Eq. (2b)]	0.006
	1.815	0.0236	0.0135	0.0270	0.0203	1.736 [Eq. (2g)]	4.366
	1.865	0.0211	0.0132	0.0343	0.0158	1.777 [Eq. (2g)]	4.710
	1.78	0.0179	0.0119	0.0417	0.0119	1.833 [Eq. (2g)]	2.977
	1.767	0.0195	0.0130	0.0390	0.0130	1.804 [Eq. (2g)]	2.076
	1.85	0.0175	0.0000	0.0263	0.0263	1.872 [Eq. (2g)]	1.200

Table 2 (*Continued*)
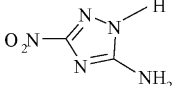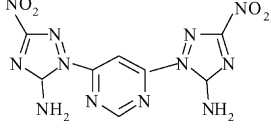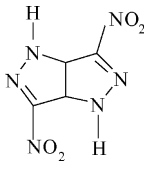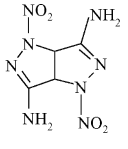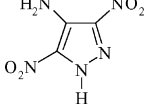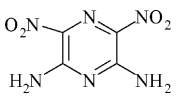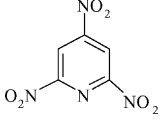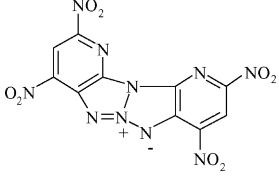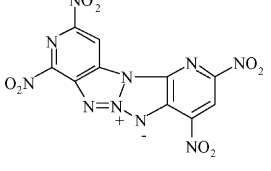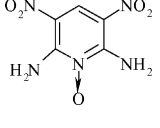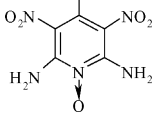
Explosive	Measured density (g/cm^3)[a]	a'	b'	c'	d'	Calculated density (g/cm^3) by new method[b]	% error
	1.819	0.0155	0.0233	0.0388	0.0155	1.890 [Eq. (2)]	3.897
	1.865	0.0211	0.0132	0.0343	0.0158	1.777 [Eq. (2g)]	4.710
	1.865	0.0202	0.0101	0.0303	0.0202	1.846 [Eq. (2)]	1.003
	1.845	0.0175	0.0175	0.0351	0.0175	1.871 [Eq. (2)]	1.407
	1.9	0.0173	0.0173	0.0289	0.0231	1.877 [Eq. (2)]	1.205
	1.84	0.0200	0.0200	0.0300	0.0200	1.856 [Eq. (2f)]	0.868
	1.876	0.0234	0.0093	0.0187	0.0280	1.803 [Eq. (2)]	3.914
	1.88	0.0256	0.0051	0.0256	0.0205	1.880 [Eq. (2b)]	0.011
	1.88	0.0256	0.0051	0.0256	0.0205	1.880 [Eq. (2b)]	0.011
	1.878	0.0233	0.0233	0.0233	0.0233	1.867 [Eq. (2c)]	0.583
	1.876	0.0217	0.0261	0.0261	0.0217	1.872 [Eq. (2c)]	0.237

Table 2 (*Continued*)

Explosive	Measured density (g/cm^3)^a	a'	b'	c'	d'	Calculated density (g/cm^3) by new method^b	% error
	1.86	0.0217	0.0087	0.0174	0.0304	1.882 [Eq. (2c)]	1.187
	1.918	0.0185	0.0185	0.0278	0.0231	1.889 [Eq. (2c)]	1.508
rms							2.318

^{a} Measured density for nitroaromatic explosives, where name of explosives are given, were taken from Ref. [35] and for new explosive compounds, where molecular structure are drawn, were obtained from Ref. [36].
^{b} Used equations are given in bracket.

where ρ_0 is the crystal density of explosive, x_1–x_4 are adjustable parameters, a', b', c' and d' are the number of carbon, hydrogen, nitrogen and oxygen divided by molecular weight of explosive, respectively. This equation provides unperturbed core correlation for estimation crystal density of a large number of nitroaromatic explosives, which requires as input only the elemental composition. Although Eq. (1) contains four adjustable parameters, the study showed that optimization of four parameters with large experimental data, by MATLAB [30], gives good result. Therefore, large number experimental crystal densities of nitroaromtic explosives, which are given in Tables 1 and 2, were used to find constant parameters of Eq. (1) as:

$$\rho_0 = 10.5739a' + 0.1266b' + 30.3796c' + 35.1850d' \quad (2)$$

Eq. (1) can also be corrected for some cases where molecular structure or intermolecular forces can cause compact or expansion of volume of compound. The corrected crystal densities correlations can be expressed for some nitroaromatic explosives according to the following classification for compounds in which contain:

(a) –N$_3$ groups attached to aromatic ring:

$$\rho_{0,\text{corr}} = -0.0238 + 0.9615\rho_0 \quad (2a)$$

(b) positive and negative charges on nitrogen:

$$\rho_{0,\text{corr}} = 1.3022 + 0.3261\rho_0 \quad (2b)$$

(c) free oxygen attached to nitrogen of heterocyclic aromatic structure:

$$\rho_{0,\text{corr}} = 1.3958 + 0.2657\rho_0 \quad (2c)$$

(d) an aromatic ring attached to –OR or –OAr, where R and Ar are alkyl and aromatic groups, respectively:

$$\rho_{0,\text{corr}} = -0.5139 + 1.2532\rho_0 \quad (2d)$$

(e) more than two –OH or more than two –NH$_2$ attached to aromatic ring:

$$\rho_{0,\text{corr}} = 1.1024\rho_0 \quad (2e)$$

(f) one –OH or two –OH or two –NH$_2$ attached to aromatic ring:

$$\rho_{0,\text{corr}} = 0.2332 + 0.8872\rho_0 \quad (2f)$$

(g) an aromatic ring connected to directly to another aromatic ring (Ar–Ar):

$$\rho_{0,\text{corr}} = -0.2164 + 1.093\rho_0. \quad (2g)$$

The priority of using equations are from Eqs. (2a)–(2g). However, for a compound such as diazodinitrophenol, Eq. (2a) should be used rather than Eq. (2f). The results of using mentioned correlations for some nitroaromatic high explosives are given in Table 1 and compared with experimental data as well as Tarver method [28]. Since group molar volumes for some group configurations have not been considered in Tarver method [28], density of some nitroaromatic compounds cannot be calculated by Tarver method [28]. Thus, Table 2 shows only comparison of the calculated density by these correlations with measured values. As seen in Table 1, root mean square deviation of the present method, 1.907, is comparable with the results of Tarver method [28], 1.546. The first 25 explosive compounds in Table 1 to which the new approach was applied only correlations (2), (2e) and (2f) are required to describe these compounds. The average error in Table 1 is 1.418% and 1.304% for new approach and Tarver method [28], respectively. The estimated density by this new approach is within 1% of the reported density for 12 explosive compounds, within 1–2% for six explosive compounds, and within 2–3% for five explosive compounds, and more than 3% for remainder five explosive compounds. The second series of explosives that are listed in Table 2 consist of 35 well-known and new synthesized explosives where Tarver method [28] cannot be applied. The average error is 1.776% in this case. Of the estimated densities, 34% are within 1% of the reported densities and another 31% are within 1–2% of reported densities.

Undoubtedly there are other nitroaromatic explosives whose densities have been measured, but the 60 explosive compounds in Tables 1 and 2 represent those obtained during a fairly extensive review in open literature. Of the estimated densities, 68.3%

are within 2% of the measured densities, with another 15% within 2–3%. The main conclusion regarding the applicability of the new approach to the density estimation is that the results are very promising. A total 60 nitroaromatic explosives were considered in the new approach, and 40% of the estimated densities were within 1% of the measured densities, 28.3% were within 1–2%, 15% were within 2–3%, 8.3% were within 3–4% and 8.3% were more than 4% different from reported densities.

One of the most important applications of density of a new explosive is to determine Chapman–Jouguet (C–J) pressure and detonation velocities, as two important detonation performance parameters, at crystal density. Since non-equilibrium effects in reaction zone may contribute to large uncertainty for determining detonation pressures by various indirect methods, detonation pressure is not easy to determine which span a range of 10–20% [31]. The search for higher energy and yet safe explosives is concentrated to a large extent on the synthesis of thermally stable molecules having mass densities greater than 1.9 g/cm^3. As an example of application the new approach for determining performance of new explosive compounds, it can be considered 2,4,6-trinitrotriazine and 3,6-dinitrotetrazine that are of the high energy density material [32–34]. There is no method reported for their synthesis [32,33]. The calculated density of these compounds by using Eq. (2) are 1.97 g/cm^3 for 2,4,6-trinitrotriazine and 2.0 g/cm^3 for 3,6-dinitrotetrazine which is near of two calculated values 1.97 and 1.98 g/cm^3 for 2,4,6-trinitrotriazine and 3,6-dinitrotetrazine by group additivity method, respectively [32]. Calculated detonation pressure [10] with estimated heat of formation 46 kcal/mol for 2,4,6-trinitrotriazine gives 389 kbar for 1.97 g/cm^3. Therefore, the results are good for large uncertainties of various methods of measuring the C–J detonation pressure in prediction of unsynthesized high explosive. Of the densities estimated in this study, all of calculated densities were less than 5.7% of the measured density and thus would yield realistic estimates of the C–J detonation pressure.

Table 3
Summary of the accuracy of new approach to density estimation

	Number of compounds within this range of density estimation error	% of compounds studied within this range
% error range		
0–1	24	40
1–2	17	28.33
2–3	9	15
3–4	5	8.33
4–5	4	6.67
>5	1	1.67
Absolute error range (g/cm^3)		
0.00–0.01	15	25
0.01–0.02	12	20
0.02–0.03	11	18.33
0.03–0.04	7	11.67
0.04–0.05	4	6.67
0.05–0.06	2	3.33
0.06–0.07	4	6.67
0.07–0.08	2	3.33
0.08–0.09	3	5

The average absolute error in density was 0.0265 g/cm^3 in Tables 1 and 2 and may represent a better indication of the accuracy of the new approach than percent errors. The absolute error in density exceeded 0.06 g/cm^3 for only 4 of 60 explosive compounds. Taking into account the greater densities and geometrical complexities of the nitroaromatic explosives, it is found that the overall agreement of the new approach with reported densities is quite good. The overall results of density estimation by this new approach for 60 nitroaromatic explosive compounds whose estimated and measured densities can be compared are summarized in Table 3.

3. Conclusions

It can be inferred from experimental data that density of nitroaromatic explosive compounds can be expressed by elemental composition of any $C_aH_bN_cO_d$ nitroaromatic explosives. Density is an important property for calculating the performance of explosives. Comparison of calculated results with experimental data listed in Tables 1–3 may be taken as appropriate validation of the new simple method for use with nitroaromatic $C_aH_bN_cO_d$ explosives. It should be noted that the new approach gives the simplest and easiest method and at the same time gives reliable results for density of nitroarmatic explosive. It is seen from Table 1 that the present method has a root mean square (rms) of deviations from experiment 1.912, while rms deviation for Tarver method [28] is 1.546 even for some explosives mentioned in Table 1 where it can be used. In this paper one core and several corrected correlations have been introduced for estimating the density of any nitroaromatic $C_aH_bN_cO_d$ explosives so that molecular structure and type of groups attached to aromatic rings can determine using the path for suitable correlation. It can feel that the introduced correlations represent a significant advance in a priori estimation of density of explosives. The results of this work are remarkable for chemist because the density of nitroaromatic explosive is readily calculated by a desk calculator of about the same reliability as one could expect from a more complex group additivity methods.

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