

Prediction of densities of acyclic and cyclic nitramines, nitrate esters and nitroaliphatic compounds for evaluation of their detonation performance

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Abstract

A novel approach to density prediction by elemental composition is developed for various important classes of explosives. Some correlations based on two different models are introduced for 82 different energetic compounds whose molecules contain functional groups common to $C_aH_bN_cO_d$ explosives. These include acyclic and cyclic nitramines, nitrate esters and nitroaliphatic compounds. Of the 69 well-known and recently new synthesized organic explosives for which direct comparison could be made with Tarver group additivity method, root mean square (rms) of deviation for 19 acyclic and cyclic nitramines is 2.839 and 3.412 while for 50 nitrate esters and nitroaliphatic explosives is 1.936 and 1.752 for new and Tarver's method, respectively. This method is the simplest procedure for calculating density of energetic compounds which gives good results as compared to well-developed group additivity method for estimation density of organic explosives.

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1. Introduction

It is determined that the energy which a detonation wave releases within and behind itself will depend upon the mass of explosive traversed per unit area of the wave. However, detonation velocity appears to be proportional to loading density. Density is an important aspect of performance behavior so that its theoretical calculations are indispensable in recognizing energetic materials of interest. Some empirical methods were recently introduced for reliable detonation and thermochemical properties of ideal and non-ideal pure or mixed explosives of different classes [1–12]. However, density of energetic material has an important role in predicting its detonation pressure and velocity. Crystalline or maximum nominal density would be usually needed to obtain the highest predicted detonation performance of any new energetic compounds, by a computer code such as CHEETAH [13] or various empirical methods [14].

The molecular structure, elemental composition, heat of formation, solid state density and microstructure are important properties characterizing the performance of an energetic mate-

rial. Microstructure shows the three-dimensional structure with various types of dislocations and imperfections. The molecular microstructures are the factors that affect the sensitivity of a material in response to impact or shock stimuli. Density of organic compounds can be calculated on the fundamental basis if all inter- or intramolecular forces are known. To calculate density of an energetic compound, the complex theoretical approach uses quantum chemistry for determining detailed information about the crystal structure [15–19]. Another convenient method for estimating the density of energetic materials is based on summing up the volume of each atom or molecular fragment [20–24]. Group or volume additivity for density predictions of energetic materials is truly a back-of-the-envelope or spread sheet calculation and involves the summation of the appropriate atom and functional group volumes to give an effective condensed-state volume for a molecule, then density.

It should be mentioned that increasing the oxygen balance and heat of formation will generally increase the sensitivity of an explosive as well as the performance. Since detonation pressure is proportional to the square of the density, increasing density should do more to improve the performance. Thus, density is one of the primary physical parameter in detonation performance [1,4]. The purpose of this work is to show some simple equations for predicting density of acyclic and

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cyclic nitramines, nitrate esters and nitroaliphatic compounds. The new correlations will be applied to some of common and recently synthesized $C_aH_bN_cO_d$ explosives. To show the reliability of predicted values as compared to well-known different additivity group methods, the method of Tarver [23] is also used for some explosives. The introduced models will be very valuable in directing research efforts towards design of complicated molecular structure of high-density explosives because the calculated density could be meaningful in the decision as to whether it is worth the effort to attempt a new and complex synthesis.

2. Determination of density of nitrate esters and nitroaliphatic compounds

One of the fundamental goals in the field of organic explosives is to develop methods for predicting the performance of new explosives before synthesis which requires the density and the heat of formation of the explosive. However, the main intent in this work was to investigate a generalized simple method for density prediction of several classes of $C_aH_bN_cO_d$ explosives. It was noticed that the results predicted by this method are comparable with more complicated quantum mechanical computations as well as group additivity procedure.

The study on acyclic and cyclic nitrate esters and nitroaliphatic systems shows the atomic composition and the number of special functional groups can be integrated into an empirical formula to predict density of proposed explosive. The general formula based on this assumption for $C_aH_bN_cO_d$ acyclic and cyclic nitrate esters and nitroaliphatic compounds can be written as

$$\rho_0 = \frac{Aa + Bb + Cc + Dd + \sum n_i(\text{FG})_i}{M_W} \quad (1)$$

where A, B, C, D and $(\text{FG})_i$ are adjustable parameters for elemental composition and specified functional groups (FG = functional group), M_W the molecular weight of the explosive, ρ_0 density of explosive, and n_i is the number of functional groups. To obtain adjustable coefficients of Eq. (1), experimental data of Table 1 were used. Since the presence of functional groups of alcohols, esters and ethers ($-\text{OH}$, $-\text{C}(=\text{O})\text{O}-$ and $-\text{O}-$) shows an appreciable effect on the molecular forces and packing of molecules in a given volume with respect to the other functional groups, the following equation can be obtained as a core correlation by optimizing adjustable coefficients for acyclic and cyclic nitrate ester and nitroaliphatic compounds:

$$\rho_0 = \frac{47.9732a - 19.2948b + 26.5340c + 26.0011d - 25.3190n_{\text{COO}} - 0.6358n_{\text{O}} + 11.5413n_{\text{OH}}}{M_W} \quad (2)$$

where n_{COO} , n_{O} and n_{OH} are the number of esters, ethers and alcohols functional groups.

Multiple linear regression method [25] was also used to find adjustable parameters. The left-division method for solving linear equations uses the least squares method because the equation set is overdetermined [25]. This correlation would be corrected

for some specific cases according to certain molecular structure as below:

(a) Mononitroalkanes:

$$\rho_{0,\text{corr}} = 0.4170 + 0.5970\rho_0 \quad (2a)$$

(b) Two $-\text{NO}_2$ groups attached to one carbon (without mentioned functional groups):

$$\rho_{0,\text{corr}} = 0.1233 + 0.8373\rho_0 \quad (2b)$$

(c) Three $-\text{NO}_2$ groups attached to one carbon:

$$\text{if } n_{\text{CH}_2} \geq 1.5n_{\text{NO}_2} \text{ then } \rho_{0,\text{corr}} = 3.033 - \rho_0 \quad (2c)$$

$$\text{if } n_{\text{CH}_2} \leq 0.6n_{\text{NO}_2} \text{ then } \rho_{0,\text{corr}} = -0.3788 + 1.2569\rho_0 \quad (2c')$$

For those molecules that satisfy both conditions b and c, Eqs. (2c) and (2c') rather than (2b) should be used.

(d) For nitrate systems (without cyclic ring attachment), if $n_{\text{CH}_2\text{ONO}_2} + n_{\text{CHONO}_2} \geq 4$:

$$\rho_{0,\text{corr}} = 0.1745 + 0.9235\rho_0 \quad (2d)$$

(e) Cage and cyclo-nitro compounds in which only one $-\text{NO}_2$ (not more) attached to carbon atom:

$$\rho_{0,\text{corr}} = -0.0515 + 0.9142\rho_0. \quad (2e)$$

3. Determination of density of cyclic and acyclic nitramine compounds

The study showed that there is no need to use the effect of the other functional groups as in Eq. (1) for cyclic and acyclic nitramines because it seems that N- NO_2 group has predominant effect in packing of molecules. Experimental data of Table 2 were used to find coefficients of Eq. (1) in this situation. Thus, two optimized new correlations for calculating density of cyclic (and the compounds in which N- NO_2 attached to an aromatic ring such as tetryl) and acyclic nitramines are introduced as the following forms, respectively:

$$\rho_{0,\text{cyclic}} = \frac{13.1466a - 5.3031b + 39.7241c + 29.3395d}{M_W} \quad (3)$$

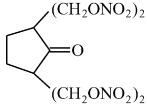
$$\rho_{0,\text{acyclic}} = \frac{66.8566a - 27.3717b + 52.9597c + 12.8071d}{M_W} \quad (4)$$

Correlation (3) can be applied only for polycyclic energetic compounds that contain no more than one oxygen in their cyclic structures.

4. Results and discussion

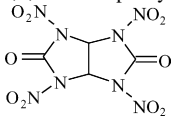
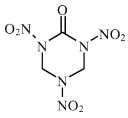
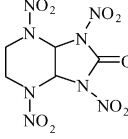
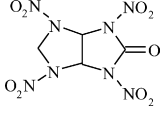
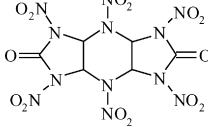
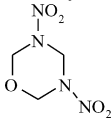
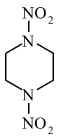
The above correlations provide a new method to estimate the density of some well-known classes of explosives, which requires as input only the elemental compositions and some specified functional groups. The output of these correlations

Table 1
Density estimation for 50 acyclic and cyclic nitrate ester and nitroaliphatic compounds by new method and Tarver method [23]

Explosive	Measured density (g/cm ³) ^a	Calculated density (g/cm ³) by new method	%error	Calculated density (g/cm ³) by Tarver method	%error
CH ₃ CH ₂ NO ₂	1.045	1.038	0.676	1.0240	2.010
CH ₃ (CH ₂) ₂ NO ₂	1.008	1.003	0.476	1.0010	0.694
CH ₃ (CH ₂) ₃ NO ₂	0.971	0.978	-0.711	0.9852	-1.462
CH ₃ (CH ₂) ₅ NO ₂	0.949	0.944	0.576	0.9642	-1.602
CH ₃ CH(NO ₂)CH ₂ CH ₃	0.985	0.978	0.721	0.9709	1.431
CH ₃ CH(NO ₂)CH ₃	0.988	1.003	-1.538	0.9842	0.385
CH ₃ CH ₂ CH(NO ₂)CH ₂ CH ₃	0.957	0.959	-0.174	0.9610	-0.418
CH ₃ CH(NO ₂) ₂	1.35	1.350	-0.015	1.3370	0.963
CH ₃ CH ₂ CH(NO ₂) ₂	1.261	1.281	-1.558	1.2710	-0.793
O ₂ NCH ₂ C(=O)OCH ₂ CH ₃	1.1953	1.218	-1.931	1.1883	0.586
CH ₃ CH ₂ ONO ₂	1.1	1.143	-3.904	1.1121	-1.100
O ₂ NOCH ₂ CH ₂ ONO ₂	1.48	1.499	-1.280	1.4847	-0.318
O ₂ NOCH ₂ CH ₂ CH(ONO ₂)CH ₂ ONO ₂	1.52	1.537	-1.124	1.5212	-0.079
O ₂ NOCH ₂ CH(ONO ₂)CH ₂ CO ₂ CH(ONO ₂)CH ₃	1.47	1.520	-3.400	1.4854	-1.048
O ₂ NOCH ₂ CH ₂ OCH ₂ CH ₂ ONO ₂	1.38	1.388	-0.551	1.4410	-4.420
O ₂ NOCH ₂ CH ₂ OCH ₂ OCH ₂ CH ₂ ONO ₂	1.33	1.357	-2.042	1.3350	-0.376
CH ₃ C(CH ₂ ONO ₂) ₃	1.47	1.489	-1.326	1.4854	-1.048
(O ₂ NOCH ₂) ₃ CCH ₂ OCH ₂ C(CH ₂ ONO ₂) ₂ CH ₂ OCH ₂ C(CH ₂ ONO ₂) ₃	1.58	1.617	-2.355	1.5679	0.766
O ₂ NOCH ₂ CH(ONO ₂)CH ₂ ONO ₂	1.596	1.591	0.341	1.5902	0.363
O ₂ NOCH ₂ (CHONO ₂) ₄ CH ₂ ONO ₂	1.73	1.729	0.074	1.7128	0.994
(CH ₂ ONO ₂) ₄ C	1.77	1.646	6.983	1.7649	0.288
(O ₂ NOCH ₂) ₃ CCH ₂ OCH ₂ OCH ₂ C(CH ₂ ONO ₂) ₃	1.63	1.625	0.314	1.6225	0.460
(CH ₂ ONO ₂) ₃ CC(CH ₂ ONO ₂) ₃	1.63	1.674	-2.709	1.6590	-1.779
O ₂ NC(CH ₂ ONO ₂) ₃	1.64	1.637	0.164	1.6400	0.000
O ₂ NCH ₂ CH ₂ NO ₂	1.46	1.465	-0.364	1.4090	3.493
O ₂ NCH ₂ CH ₂ CH ₂ NO ₂	1.353	1.382	-2.161	1.3290	1.774
CH ₃ C(NO ₂) ₂ CH ₂ CO ₂ (CH ₂) ₂ CO ₂ CH ₂ C(NO ₂) ₂ CH ₃	1.51	1.511	-0.050	1.5173	-0.483
HOCH ₂ CH ₂ NO ₂	1.27	1.270	0.018	1.2900	-1.575
CH ₃ CH(NO ₂)CH ₂ OH	1.1841	1.190	-0.484	1.1964	-1.039
O ₂ NOCH ₂ CH(OH)CH ₂ ONO ₂	1.523	1.510	0.873	1.5490	-1.707
C ₂ H ₅ CH(NO ₂)CH ₂ OH	1.1332	1.129	0.398	1.1506	-1.535
CH ₃ C(NO ₂) ₂ CH ₃	1.3	1.281	1.488	1.3120	-0.923
C(NO ₂) ₃ CH ₂ CO ₂ (CH ₂) ₈ CO ₂ CH ₂ C(NO ₂) ₃	1.45	1.450	-0.027	1.4980	-3.310
C(NO ₂) ₃ CH ₂ CO ₂ (CH ₂) ₇ CO ₂ CH ₂ C(NO ₂) ₃	1.475	1.475	0.014	1.5262	-3.471
C(NO ₂) ₃ CH ₂ CO ₂ (CH ₂) ₆ CO ₂ CH ₂ C(NO ₂) ₃	1.59	1.583	0.436	1.5571	2.069
C(NO ₂) ₃ CH ₂ CO ₂ (CH ₂) ₅ CO ₂ CH ₂ C(NO ₂) ₃	1.63	1.609	1.266	1.5911	2.387
HC[OCH ₂ C(NO ₂) ₃] ₃	1.8	1.861	-3.405	1.8334	-1.856
H ₂ C[OCH ₂ C(NO ₂) ₃] ₂	1.72	1.797	-4.455	1.7263	-0.366
C(NO ₂) ₃ (CH ₂) ₂ CO ₂ (CH ₂) ₂ CO ₂ (CH ₂) ₂ C(NO ₂) ₃	1.63	1.637	-0.443	1.6288	0.074
C(NO ₂) ₃ CH ₂ CO ₂ (CH ₂) ₄ CO ₂ CH ₂ C(NO ₂) ₃	1.64	1.637	0.169	1.6288	0.683
C(NO ₂) ₃ CH ₂ CO ₂ CH ₂ CO ₂ CH ₂ C(NO ₂) ₃	1.75	1.798	-2.728	1.7713	-1.217
C(NO ₂) ₃ (CH ₂) ₂ CO ₂ CH ₂ C(NO ₂) ₃	1.767	1.736	1.774	1.7566	0.589
C(NO ₂) ₃ CH ₂ CO ₂ (CH ₂) ₃ CO ₂ CH ₂ C(NO ₂) ₃	1.67	1.667	0.193	1.6709	-0.054
(O ₂ N) ₃ CC(NO ₂) ₃	1.998	1.997	0.029	2.0040	-0.300
C(NO ₂) ₃ (CH ₂) ₂ CO ₂ CH ₂ C(NO ₂) ₂ CH ₃	1.68	1.680	-0.006	1.6404	2.357
CH ₃ C(NO ₂) ₂ CH ₂ CO ₂ CH=CHCO ₂ CH ₂ C(NO ₂) ₂ CH ₃	1.6	1.620	-1.266	1.5530	2.938
CH ₃ C(NO ₂) ₂ CH ₂ CO ₂ CH=CH ₂	1.47	1.431	2.657	1.4333	2.497
C ₂ H ₅ CO ₂ (CH ₂) ₂ C(NO ₂) ₂ CH ₃	1.28	1.309	-2.281	1.2777	0.180
HOCH ₂ C(CH ₂ ONO ₂) ₃	1.54	1.540	-0.005	1.5698	-1.935
	1.62	1.678	-3.582	1.6200	0.000
Average deviation			1.292		1.309
rms deviation			1.958		1.752

^a Measured densities were obtained from Ref. [23].

Table 2
Density estimation for 19 cyclic and acyclic nitramines compounds by new method and Tarver method [23]

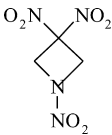
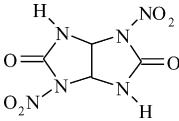
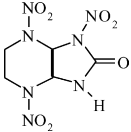
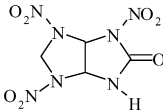
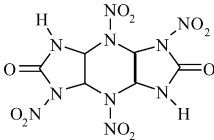

Explosive	Measured density (g/cm ³) ^a	Calculated density (g/cm ³) by new method	%error	Calculated density (g/cm ³) by Tarver method	%error
(CH ₃) ₂ NNO ₂	1.1090	1.122	-1.209	1.1750	-5.951
(C ₂ H ₅) ₂ NNO ₂	1.0570	1.061	-0.415	1.0500	0.662
CH ₃ N(NO ₂)(CH ₂) ₂ N(NO ₂)CH ₃	1.4460	1.443	0.238	1.3940	3.596
(C ₃ H ₇) ₂ NNO ₂	0.9950	1.024	-2.891	1.0160	-2.111
(C ₄ H ₉) ₂ NNO ₂	0.9620	0.998	-3.768	0.9942	-3.347
[(CH ₃) ₂ CH] ₂ NNO ₂	1.1040	1.024	7.268	1.1040	0.000
[(NO ₂) ₃ CCH ₂] ₂ NNO ₂	1.96	1.961	-0.057	1.9324	1.408
Tetryl (<i>N</i> -methyl- <i>N</i> -nitro-2,4,6-trinitroaniline)	1.73	1.738	-0.471	1.7390	-0.520
Ethyltetryl	1.63	1.666	-2.193	1.5780	3.190
2,4,6-Trinitrophenylnitraminoethyl nitrate	1.75	1.753	-0.147	1.8610	-6.343
	2.04	2.028	0.565	2.0290	0.539
	1.932	1.957	-1.315	1.9670	-1.812
	1.969	1.912	2.879	1.8340	6.856
	1.91	1.991	-4.240	1.8820	1.466
	2.05	2.019	1.490	1.9180	6.439
HMX	1.903	1.901	0.110	1.8500	2.785
RDX (cyclomethylenetrinitramine)	1.806	1.901	-5.255	1.7800	1.440
	1.824	1.760	3.529	1.8240	0.000
	1.638	1.627	0.649	1.6430	-0.305
Average deviation			2.036		2.567
rms deviation			2.839		3.412

^a Measured density for cyclic and acyclic nitramines were taken from Ref. [23] except for new explosive compounds that were taken from Ref. [27].

for some acyclic and cyclic nitramines, nitrate esters and nitroaliphatic systems are given in Tables 1 and 2 and compared with experimental data as well as Tarver method [23]. The results in Table 3 compares the calculated density by these correlations with measured values for some cases where Tarver method [23] cannot be applied. As seen in Table 1, root mean square (rms) deviation of the present method, 1.936, is compa-

table with the results of Tarver method 1.752 [23]. Based on the average density 1.442 g/cm³ in Table 1, the average error is 1.292% and 1.309% for both new approach and Tarver method [23], respectively. The average error in Table 2 is also 2.036% and 2.567%, which represent 0.031 and 0.077 g/cm³ based on the average density 1.622 g/cm³ for new approach and Tarver method [23], respectively. The second series of explosives that

Table 3
Density estimation for 13 acyclic and cyclic nitramines, nitrate esters and nitroaliphatic compounds by new method

Explosive	Measured density (g/cm ³) ^a	Calculated density (g/cm ³) by new method	% error
CL-20	2.04	2.000	1.980
	1.84	1.839	0.034
	1.98	1.921	2.962
	1.84	1.849	-0.466
	1.905	1.937	-1.697
	1.97	1.952	0.935
Tetranitrocubane	1.814	1.947	-7.314
Pentanitrocubane	1.959	1.945	0.703
Heptanitro cubane	2.028	1.943	4.180
Octanitrocubane	1.979	1.943	1.843
c-C ₅ H ₉ NO ₂	1.0776	1.099	-2.000
c-C ₆ H ₁₁ NO ₂	1.061	1.041	1.907
	1.83	1.817	0.700
Average deviation			2.055
rms deviation			2.769

^a Measured density for acyclic and cyclic nitramines, nitrate esters and nitroaliphatic compounds were taken from Ref. [23] except for new energetic compounds that were taken from Ref. [27].

are listed in Table 3 consist of 13 mainly new synthesized explosives where Tarver method [23] cannot be applied. The average error is 2.055%, which represents 0.037 g/cm³ based on the average density of 1.794 g/cm³. A total of 82 some acyclic and cyclic nitramines, nitrate esters and nitroaliphatic systems were considered in the new method, and 48.8% of the estimated densities were within 1% of the measured densities, 22% were within 1–2%, 13.4% were within 2–3%, 7.3% were within 3–4% and 8.5% were more than 4% different from reported densities. The average absolute error in density was 0.029 g/cm³ as shown in Tables 1–3 and the absolute error in density exceeded 0.06 g/cm³ for only 9 of 82 explosive compounds. By considering the greater densities and geometrical complexities of acyclic and cyclic nitramines, nitrate esters and nitroaliphatic systems, it is found

that the overall agreement of the new approach with reported densities is quite good.

Certain structural parameters such as high symmetry, optimum number of quaternary and/or tertiary carbons, tertiary nitrogens and condensed rings are known to maximize density. More powerful explosives can be obtained by designing energetic molecules so that the atoms are bound together in compact strained rings. These small scale molecules provide additional latent strain energy as well as high density. Polycyclic caged molecules are the most high-density molecular arrangement [25]. Polycyclic nitramine explosives such as hexanitrohexaazaadamantane (Fig. 1) and hexanitrohexaazawurtzitane (Fig. 2) have the desired structural features leading to high energy and high density.

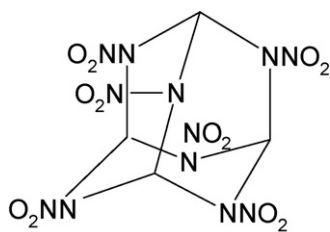


Fig. 1. The molecular structure of hexanitrohexaazaadamantane.

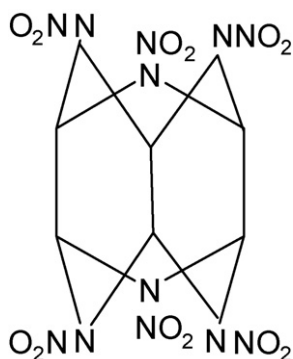


Fig. 2. The molecular structure of hexanitrohexaazawurtzitane.

Calculated densities of hexanitrohexaazaadamantane and hexanitrohexaazawurtzitane by correlation (3) lead to 2.088 and 2.000 g/cm³ values, respectively, which are consistent with calculated values by group additivity method [26] namely 2.1 g/cm³ for both explosives. The values of detonation pressure and velocity as two important detonation performance parameters strongly depend on density. Since the detonation pressure at the shockwave front is proportional to the square of the density, a slight change can significantly increase the energy of an explosive. Although the two mentioned explosives show higher performance with respect to HMX (cyclotetramethylenetetranitramine), their high sensitivity is a drawback of mentioned explosives because method of Keshavarz and Pouretedal [11] gives impact sensitivity 5 and 10 cm for hexanitrohexaazaadamantane and hexanitrohexaazawurtzitane, respectively.

5. Conclusions

An empirical methodology has been developed that uses only elemental compositions and the number of some specific functional groups to predict density of some classes of energetic compounds. The main categories of energetic compounds used were species having nitro groups attached to carbon (nitroaliphatics), oxygen (nitrate ester) and nitrogen (nitramines). As indicated in Tables 1 and 2, there are relatively large deviations in some cases for both new and Tarver methods [23] which may be attributed to intermolecular forces. As seen in Table 2, the new method for cyclic and acyclic nitramine energetic compounds is more consistent with experimental data with respect to Tarver method [23].

Although quantum mechanical computations have a stronger theoretical basis for predictions of density than proposed here,

those computations are complex and also require special software. The methodology presented here has the advantage that it gives the simplest and easiest method and at the same time gives reliable results for density of some acyclic and cyclic nitramines, nitrate esters and nitroaliphatic systems. The results of the new correlations show that this methodology to predict density of acyclic and cyclic nitramines, nitrate esters and nitroaliphatic systems is reasonably acceptable tool to be used in the rapid assessment and screening of notional energetic materials.

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