

# Theoretical prediction of condensed phase heat of formation of nitramines, nitrate esters, nitroaliphatics and related energetic compounds

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Received 28 September 2005; received in revised form 6 December 2005; accepted 6 December 2005

Available online 19 January 2006

## Abstract

An empirical approach is presented for calculation heats of formation of nitramines, nitrate esters, nitroaliphatics and related energetic compounds which contain at least one of the functional groups including N-NO<sub>2</sub>, C-ONO<sub>2</sub> or nonaromatic C-NO<sub>2</sub>. This approach is based on elemental composition and various structural and functional group parameters of C<sub>a</sub>H<sub>b</sub>N<sub>c</sub>O<sub>d</sub> energetic compounds. Heat of formation for 78 nitrocompounds including nitramines, nitrate esters, nitroaliphatics and the data obtained is compared with experimental data. Root mean square (rms) of deviation for 19 well known of mentioned energetic compounds are also compared with complex quantum mechanical computations which show 23.8 and 21.3 kJ/mol for new and quantum mechanical methods, respectively. Predicted condensed phase heats of formation for remainder 59 energetic molecules with complex molecular structures have a rms deviation from experiment of 42.3 kJ/mol.

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**Keywords:** Condensed phase heat of formation; Nitramines; Nitrate esters; Nitroaliphatic compounds

## 1. Introduction

The study of an energetic system by theoretical methods has accelerated dramatically because they provided a considerable insight into the understanding of factors affecting their behavior. Theoretical methods for predicting detonation parameters of new energetic materials can reduce costs associated with synthesis, test and evaluation of the materials, which are cost-effective, environmentally desirable and time-saving capabilities at the early stages of development.

Heat of formation is a measure of energy content of an energetic material that can decompose, ignite and explode by heat and impact. It enters into the calculation of explosive and propellant properties such as detonation velocity [1], detonation pressure [2], heat of detonation [3] and specific impulse [4]. Group additivity methods and quantum mechanics are two broadly methods for calculation gas phase heat of formation. Condensed phase heat of formation can be calculated by mentioned methods through combining heats of vaporization and sublimation. A different complex scheme has also been recently introduced

for calculation heats of formations of some explosives in the range  $Q_{\text{corr}} > 4602$  kJ/g [5], where  $Q_{\text{corr}}$  is the corrected heat of detonation of Kamlet's method [6].

Thermochemical codes such as TIGER [7] by using condensed phase heat of formation of energetic material and equations of state for detonation products can estimate detonation parameters of explosives. Some well-known equations of state are Becker–Kistiakosky–Wilson (BKW) [8] and the Jacobs–Cowperthwaite–Zwisler (JCZ) [9,10] and Kihara–Hikita–Tanaka (KHT) [11]. To find various reliable detonation parameters, some empirical methods have been recently introduced [1–4,12–20], which usually require heats of formation of energetic materials as one of the essential parameters.

The paper presents a new simple scheme for obtaining condensed phase heats of formation of nitramines, nitrate esters, nitroaliphatics and related energetic compounds as important classes of energetic materials. The main intent was to investigate the likelihood of obtaining the simplest procedure respect to available methods for calculating condensed phase heats of formation of mentioned energetic materials. To show the reliability of predicted condensed phase heats of formation values, the results for 76 nitrocompounds including nitramines, nitrate esters, nitroaliphatics and the heat of formation values obtained in the present investigation are compared with the experimental

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data. Some of mentioned energetic compounds are also compared to complex quantum mechanical method of Rice et al. [21] where computed values were available. The introduced correlation will be very valuable in directing research efforts towards design of high “energy content” organic molecules. This leads the chemist in the quick decision as to whether it is worth the effort to attempt a new and complex synthesis.

## 2. Group additivity and quantum mechanical methods

Group additivity methods are useful in chemistry so that the properties of the molecules can be derived from atoms or functional groups from which they are made. Benson and Joback methods are two group additivity methods which commonly used to estimate thermochemical quantities of various organic molecules [22]. Joback’s method assigns incremental heat of formation values to the ideal gas phase of common functional groups such as  $-\text{CH}_3$ ,  $>\text{C}=\text{O}$ ,  $\text{OH}$  and so on. Benson’s method incorporate the effects of second-nearest neighbors that produces more reliable values of gas phase heats of formation at the greater complexity.

There have been developments for quantum mechanics in density functional theory (DFT) for calculating molecular energies so that they provide near chemical accuracy for quantities such as bond strengths and heats of formation of energetic compounds. Sana et al. [23] used quantum mechanics to introduce the concept of stabilization energy which measures the special effects due to bond interaction, electron dislocation, etc. This method pointed out that  $\text{NO}_2$  constituent produces larger destabilization energy. Many macroscopic properties of bulk

energetic materials can be determined from quantum mechanical information calculated for isolated molecules. Politzer and coworkers [24–32] have established the quantum mechanical electrostatic calculations of the isolated molecule to determine aqueous solvation free energies, lattice energies in ionic crystals, diffusion coefficients, solubilities, boiling points, partition coefficients, critical constants and impact sensitivities. Rice and coworkers [21,33] utilized these ideas to predict heats of formation of energetic materials in the gas, liquid and solid state as well as heats of detonation from quantum mechanical computation of isolated molecule. They used generalized gradient approximation of DFT characterization using the 6-31G\* basis set [34] and hybrid B3LYP DFT as well as the method atom equivalents [35,36] for converting quantum mechanical energies of molecules to gas phase heats of formation. To calculate condensed phase heats of formation, they also used surface electrostatic potentials of individual molecules for computation of heats of sublimation and vaporization as recommended by Politzer and coworkers [28,30,32].

## 3. New scheme for obtaining condensed phase heats of formation of nitramines, nitrate esters, nitroaliphatics and related energetic compounds

Condensed phase heat of formation of an energetic compound can be related to its molecular structures. The study of various  $\text{C}_a\text{H}_b\text{N}_c\text{O}_d$  nitramines, nitrate esters, nitroaliphatics and related energetic compounds showed that elemental composition and some special structural factors can be related to their values of condensed phase heat of formation. The results indicated that the

Table 1  
Comparison of theoretically predicted heats of formation (kJ/mol) with experimental and quantum mechanical computed data

No.	Name	Experiment <sup>a</sup>	Quantum mechanical <sup>b</sup>	DEV <sup>c</sup>	New method	DEV <sup>c</sup>
1	Nitromethane	−112.5	−114.6	2.1	−102.9	−9.6
2	Dinitromethane	−104.9	−96.2	−8.8	−108.4	3.3
3	Trinitromethane	−68.0	−45.2	−23.0	−113.8	45.6
4	Tetranitromethane	38.5	38.1	0.4	46.4	−7.9
5	Nitroethane	−143.9	−155.2	11.3	−137.2	−6.7
6	Hexanitroethane	108.4	101.7	6.7	92.5	15.9
7	1-Nitropropane	−167.4	−180.3	13.0	−171.1	3.8
8	2-Nitropropane	−180.3	−189.1	8.8	−171.1	−9.2
9	1-Nitrobutane	−192.6	−202.9	10.5	−205.0	12.6
10	2-Nitrobutane	−207.6	−210.9	3.3	−205.0	−2.5
11	2-Methyl-2-nitropropane	−229.7	−225.1	−4.6	−205.0	−24.7
12	Ethyl nitrate	−190.4	−203.3	13.0	−197.5	7.1
13	Nitroglycerine	−369.9	−370.7	0.8	−363.6	−6.3
14	<i>n</i> -Propyl nitrate	−214.6	−227.2	12.6	−231.8	17.2
15	Tetranitrate pentaerythritol	−538.5	−566.1	27.6	−497.5	−41.0
16	Nitroguanidine	−86.6	−31.0	−55.6	−79.9	−6.7
17	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	75.3	87.0	−11.7	135.6	−60.2
18	Hexahydro-1,3,5-trinitrotriazine	79.1	107.1	−28.0	101.7	−22.6
19	<i>N</i> -Methyl- <i>N</i> ,2,4,6-tetranitroaniline	41.0	−7.1	48.1	4.6	36.4
	rms deviation			21.3		23.8

<sup>a</sup> All experimental data taken from NIST chemistry web book [38] so that references for individual molecules are given therein.

<sup>b</sup> All quantum mechanical computation values taken from Ref. [21].

<sup>c</sup> Difference (in kJ/mol) between experimental and theoretically predicted values.

Table 2  
Comparison of predicted heats of formation (kJ/mol) with the experimental data

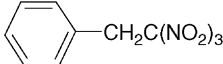
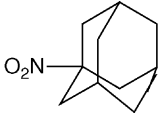
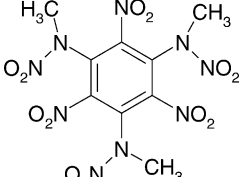
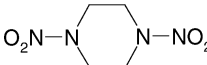
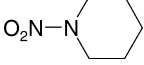
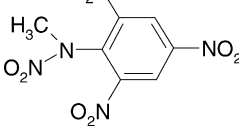
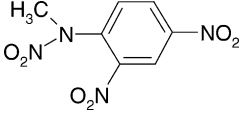
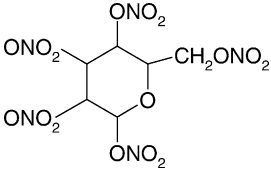
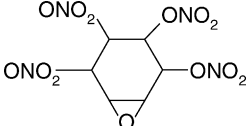
No.	Energetic compound	Experiment <sup>a</sup>	New method	DEV <sup>b</sup>
1	$\text{CH}_3\text{CH}_2\text{CH}(\text{NO}_2)_2$	-163.2	-176.6	13.4
2	$\text{O}_2\text{NCH}_2\text{CH}_2\text{NO}_2$	-178.7	-142.7	-36.0
3	$\text{O}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{NO}_2$	-207.1	-176.6	-30.5
4	$\text{HOCH}_2\text{C}(\text{NO}_2)(\text{CH}_2\text{OH})\text{CH}_2\text{OH}$	-742.2	-743.9	1.7
5	$\text{HOCH}_2\text{C}(\text{CH}_3)_2\text{NO}_2$	-410.2	-384.9	-25.3
6	$\text{C}(\text{NO}_2)_3\text{CH}_2\text{OH}$	-261.1	-327.2	66.1
7	$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_2\text{OH})_2\text{NO}_2$	-601.2	-598.3	-2.9
8	$(\text{HOCH}_2)_2\text{C}(\text{NO}_2)(\text{CH}_3)$	-570.5	-564.4	-6.1
9	$\text{C}(\text{NO}_2)_3\text{CH}_2\text{OCH}_2\text{C}(\text{NO}_2)_3$	-402.1	-447.3	45.2
10	$\text{C}(\text{NO}_2)_3\text{CH}_2\text{CH}_2\text{C}(=\text{O})\text{OCH}_2\text{C}(\text{NO}_2)_3$	-496.2	-463.2	-33.0
11	$\text{O}_2\text{NCH}_2\text{CH}_2\text{OH}$	-350.6	-316.7	-33.9
12	$(\text{CH}_3)_2\text{C}(\text{NO}_2)_2$	-192.5	-176.6	-15.9
13	$\text{O}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	-215.5	-239.3	23.8
14		-18.4	-97.1	78.7
15		-254.3	-218.4	-35.9
16		118.0	111.7	6.3
17		-53.1	-0.4	-52.7
18		-92.9	-102.1	9.2
19	$\text{CH}_3\text{CH}_2\text{N}(\text{NO}_2)\text{CH}_2\text{CH}_3$	-105.9	-131.8	25.9
20	$(\text{CH}_3)_2\text{NNO}_2$	-71.1	-64.0	-7.1
21	$\text{CH}_3\text{N}(\text{NO}_2)_2$	1.7	-35.1	36.8
22		10.5	-29.3	39.8
23		16.2	10.0	6.2
24	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{N}(\text{NO}_2)\text{CH}_2\text{CH}_2\text{ONO}_2$	-192.5	-265.7	73.2
25	$\text{CH}_3\text{CH}_2(\text{NNO}_2)\text{CH}_2\text{CH}_2\text{ONO}_2$	-164.0	-197.9	33.9
26	$\text{O}_2\text{NCH}_2\text{CH}_2\text{N}(\text{NO}_2)\text{CH}_2\text{CH}_2\text{ONO}_2$	-257.4	-263.6	6.2
27	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{N}(\text{NO}_2)\text{CH}_2\text{CH}_2\text{ONO}_2$	-206.7	-300.0	93.3
28	$\text{CH}_3\text{CH}_2\text{CH}_2\text{N}(\text{NO}_2)\text{CH}_2\text{CH}_2\text{ONO}_2$	-174.1	-231.8	57.7
29		-826.3	-761.5	-64.9
30		-444.3	-494.5	50.2

Table 2 (Continued)

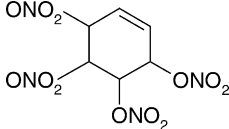
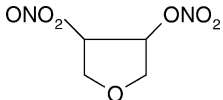
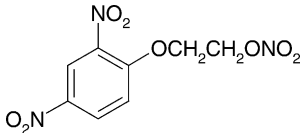
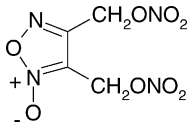
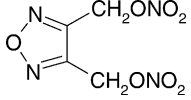
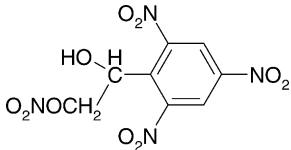
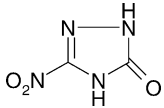
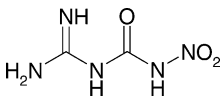
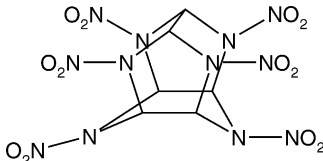
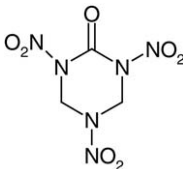
No.	Energetic compound	Experiment <sup>a</sup>	New method	DEV <sup>b</sup>
31	$\text{O}_2\text{NOCH}_2\text{CH}(\text{OH})\text{CH}_2\text{ONO}_2$	-477.0	-477.0	0.0
32	$\text{HOCH}_2\text{CH}(\text{OH})\text{CH}_2\text{ONO}_2$	-577.0	-590.8	13.8
33	$\text{O}_2\text{NOCH}_2\text{CH}(\text{ONO}_2)\text{CH}_2\text{CH}_2\text{ONO}_2$	-414.2	-397.5	-16.7
34	$\text{O}_2\text{NOCH}_2\text{CH}_2\text{ONO}_2$	-232.6	-263.6	31.0
35	$\text{O}_2\text{NOCH}_2\text{CH}(\text{ONO}_2)\text{CH}_3$	-297.1	-297.5	0.4
36	$(\text{O}_2\text{NOCH}_2)_3\text{CCH}_3$	-450.2	-431.4	-18.8
37	$\text{O}_2\text{NOCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{ONO}_2$	-274.1	-331.4	57.3
38	$(\text{O}_2\text{NOCH}_2)_3\text{CCH}_2\text{CH}_3$	-479.9	-465.7	-14.2
39	$\text{CH}_3\text{CH}(\text{ONO}_2)\text{CH}_2\text{CH}(\text{ONO}_2)\text{CH}_3$	-385.8	-365.7	-20.1
40	$(\text{O}_2\text{NOCH}_2)_2\text{C}(\text{NO}_2)\text{CH}_2\text{CH}_3$	-367.4	-371.1	3.7
41		-387.9	-404.2	16.3
42	$\text{CH}_3\text{C}(=\text{O})\text{ONO}_2$	-331.0	-270.3	-60.7
43	$(\text{O}_2\text{NOCH}_2)_3\text{CCH}_2\text{OCH}_2\text{C}(\text{CH}_2\text{ONO}_2)_3$	-979.5	-889.9	-89.6
44	$\text{O}_2\text{NOCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{ONO}_2$	-656.9	-581.2	-75.7
45	$\text{O}_2\text{NOCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{ONO}_2$	-451.0	-422.2	-28.8
46	$\text{HOCH}_2\text{CH}(\text{ONO}_2)\text{CH}_2\text{OH}$	-567.8	-590.8	23.0
47	$\text{HOCH}_2\text{CH}(\text{ONO}_2)\text{CH}_2\text{ONO}_2$	-472.4	-477.0	4.6
48	$\text{O}_2\text{NOCH}_2\text{CH}(\text{ONO}_2)\text{CH}(\text{ONO}_2)\text{CH}(\text{ONO}_2)\text{CH}(\text{ONO}_2)$	-708.8	-663.2	-45.6
49	$\text{CH}_3\text{CH}(\text{ONO}_2)\text{CH}_3$	-229.7	-231.8	2.1
50		-386.0	-358.6	-27.6
51		-298.8	-248.5	-50.3
52	$(\text{O}_2\text{NOCH}_2)_2\text{C}(\text{NO}_2)\text{CH}_3$	-374.0	-336.8	-37.2
53		-43.1	-97.1	54.0
54		-47.7	-6.3	-41.4
55		-287.7	-342.7	55.0
56		-129.4	-38.1	-91.3
57		-302.5	-367.4	64.9
58		377.4	394.1	-16.7

Table 2 (Continued)

No.	Energetic compound	Experiment <sup>a</sup>	New method	DEV <sup>b</sup>
59	 rms deviation	-41.8	-42.7	0.9
				42.3

<sup>a</sup> All experimental data taken from NIST chemistry web book [38] so that references for individual molecules are given therein.

<sup>b</sup> Difference (in kJ/mol) between experimental and mentioned values.

following equation can provide the suitable pathway to obtain a generalized correlation:

$$\Delta H_f(c) = z_1a + z_2b + z_3c + z_4d + \sum_{i=5}^n z_i n_{SF_i} \quad (1)$$

where  $\Delta H_f(c)$  is the condensed phase heat of formation,  $z_1$  to  $z_n$  the adjustable parameters and  $n_{SF_i}$  are the number of some important structural factors. Some functional groups such as OH, N-NO<sub>2</sub>, >C=O and O-NO<sub>2</sub> as well as the other parameters have predominant effects in the values of  $\Delta H_f(c)$ . To investigate the important structural factors, experimental data of various C<sub>a</sub>H<sub>b</sub>N<sub>c</sub>O<sub>d</sub> nitramines, nitrate esters, nitroaliphatics and related energetic compounds, which are listed in Tables 1 and 2, were used. The results showed that the important structural factors can be expressed as below:

$$\Delta H_f(c) = z_1a + z_2b + z_3c + z_4d + z_5n_{OH} + z_6n_{N-NO_2} + z_7n_{>C=O} + z_8n_1^0 + z_9n_{=C=N} + z_{10}n_{O-NO_2} \quad (2)$$

where  $n_{OH}$ ,  $n_{N-NO_2}$ ,  $n_{>C=O}$  and  $n_{O-NO_2}$  are the number of specified functional groups,  $n_1^0$  is equal to 0 and 1 for existence of hydrogen in molecule and hydrogen free compound respectively,  $n_{=C=N}$  the number of structural moiety  $=C=N$  in the energetic compound. The method of Kamlet and Hurwitz [37] were used for determining the parameters of Eq. (2). Optimized correlation can be given as

$$\Delta H_f(c) = 29.68a - 31.85b + 144.2c - 88.84d - 88.84n_{OH} - 39.14n_{N-NO_2} - 45.62n_{>C=O} + 256.3n_1^0 - 380.5n_{=C=N} + 30.20n_{O-NO_2} \quad (3)$$

where  $\Delta H_f(c)$  is expressed in kJ/mol. To test the validity of the correlation, the condensed phase heats of formation for 76 nitro-compounds including nitramines, nitrate esters, nitroaliphatics and the heat of formation values obtained in the present investigation are compared with the experimental data and given in Tables 1 and 2. As indicated in Table 1, the results for some mentioned energetic compounds are also compared to complex quantum mechanical method [21]. The rms deviation of the new method from experiment is 23.8 kJ/mol, which is close to the rms deviation value 21.3 kJ/mol of computed values of Rice et al. [21]. The rms deviation of the new method from experi-

ment for remainder 59 energetic compounds, given in Table 2, is 42.3 kJ/mol. Since different values for condensed phase heats of formation from different sources exist for energetic molecules, e.g. -32.13 to -77.95 kJ/mol for trinitromethane, the latest reported values of the NIST Chemistry Web Book [38], that are given in Tables 1 and 2, were taken for comparison the mentioned method with experimental data. As seen in Tables 1 and 2, there are some molecular structures of nitramines, nitrate esters, nitroaliphatics and related energetic compounds such as *N*-methyl-*N*,2,4,6-tetranitroaniline (Tetryl) in which some of NO<sub>2</sub> groups are also attached to aromatic ring. Eq. (3) can also be used in these cases with no difficulty.

The new method can be applied for any new C<sub>a</sub>H<sub>b</sub>N<sub>c</sub>O<sub>d</sub> nitramines, nitrate esters, nitroaliphatics and related energetic compounds. As seen in Table 2, the calculated heats of formation by Eq. (3) for two new explosives CL-20 and K-6 are 394.1 and -42.7 kJ/mol respectively which are close to experimental values of 377.4 [39] and -41.8 kJ/mol [40].

#### 4. Conclusions

Condensed phase heat of formation of an energetic compound is one of the essential parameters of somewhat more practical importance to the explosive user. The present method, apart from being developed as predictive tools, can provide the simplest procedure for estimating condensed phase heats of formation of organic nitramines, nitrate esters, nitroaliphatics and related energetic compounds. The method shows reasonably reliable predictions as compared to complex quantum mechanical computations. The present method may be appealing and the results are very promising because it requires as input only structural formula of nitramines, nitrate esters, nitroaliphatics and related energetic compounds.

#### Acknowledgement

This research was supported in part by Institute of Chemical and Science Technology-Tehran-Iran Research Council (Grant No. ICST-8I03-2121).

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