



Improved prediction of heats of sublimation of energetic compounds using their molecular structure

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ABSTRACT

A simple method is used to predict heats of sublimation of energetic compounds, which include nitroaromatics, nitramines, nitroaliphatics and nitrate esters. Molecular weight, some specific functional groups and structural parameters are fundamental factors in the new model. The root-mean-square deviation (rms) from experiment has been calculated for the predicted results of 92 different compounds. The calculated results for 15 compounds are also compared with complicated quantum mechanical computations, where computed outputs were available. The rms deviations of new correlation and reported quantum mechanical method are 9.9 and 13.8 kJ/mol, respectively. The present method improves earlier efforts of previous models through its application for important classes of energetic compounds, which contain the energetic bonds Ar–NO₂, N–NO₂, C–NO₂ and C–O–NO₂.

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1. Introduction

For notional energetic compounds, apart from safety problems, significant resources could be expended in their synthesis to discover upon measuring some key properties such as density and the condensed phase heat of formation. The screening of a hypothetical energetic material through reliable predictive methods allows experimental researchers to expend resources on those molecules that have desired thermodynamic and physical properties as well as enhanced performance and reduced sensitivity. Some reliable simple methods have been recently introduced to predict different thermodynamic aspects of energetic compounds such as the condensed phase heat of formation [1–5] and enthalpy of fusions [6,7].

Heat of sublimation is the best parameter concerning the characterization of the intensity of intermolecular interactions within a crystal. According to Hess's law [8], it can also be combined by the predicted gas phase heat of formation to calculate solid phase heat of formation. Experimental data of heats of sublimation of energetic are rare because the respective values of many energetic materials have not been published yet. Two simple approaches have been recently introduced to predict heats of sublimation of nitroaromatic and nitramine compounds [9,10]. These methods cannot be used for nitroaliphatics and nitrate esters. Moreover, some energetic

compounds have multifunctional energetic groups for which these methods cannot give reliable results. The purpose of this work is to introduce a reliable simple method for predicting heats of sublimation of important classes of energetic compounds, which include nitroaliphatics, nitroaromatics, nitramines and nitrate esters. In contrast to previous methods [9,10], the new correlation can also be applied to energetic compounds that have multifunctional energetic groups. Moreover, it will be shown that the present method can also be applied to halogenated energetic compounds. The predicted results will be compared with the computed results of complex quantum mechanical method [11]. It will be shown that the present method gives the simplest and easiest procedure and at the same time gives reliable results with respect to complicated quantum mechanical computations.

2. Theory

Heat of sublimation of a desired compound may be considered to be the sum of its heat of fusion and heat of vaporization, even though liquid cannot exist at the pressure and temperature in question. Thus, one might estimate heat of fusion and heat of vaporization separately and obtain heat of sublimation as the sum. Since the sublimation pressures at the melting point known are rare, using the Clausius–Clapeyron equation is difficult to obtain heat of sublimation from solid vapor pressure data [12].

Since the condensed phase for most energetic compounds is solid, the gas phase heat of formation ($\Delta H_f(g)$) and heat of sublimation (ΔH_{sub}) according to Hess's law of constant heat summation

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Table 1

Comparison of predicted heats of sublimation (kJ/mol) of nitroaromatics, nitramines, nitroaliphatics and nitrate esters with the experimental data.

Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
Nitroaromatics including polynitro arenes and polynitro heteroarenes			
	79.1 [22]	74.7	4.4
	100.9 [22]	104.5	-3.6
	107.1 [22]	99.9	7.2
	96.2 [22]	98.5	-2.3
	104.6 [22]	102.8	1.8
	105.1 [23]	114.8	-9.7
	82.9 [22]	98.5	-15.6
	78.6 [22]	82.2	-3.6
	103.3 [22]	106.5	-3.2
	98.3 [22]	102.3	-4.0
	101.9 [22]	110.8	-8.9
	101.3 [22]	98.0	3.3
	120.8 [22]	119.1	1.7
	112.1 [22]	102.8	9.3

Table 1 (Continued)

Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
	110.0 [22]	108.2	1.8
	92.7 [22]	98.0	-5.3
	100.4 [22]	101.8	-1.4
	107.9 [22]	111.5	-3.6
	129.8 [23]	118.0	11.8
	107.9 [22]	118.5	-10.6
	115.0 [22]	116.0	-1.0
	179.9 [23]	173.7	6.2
	111.2 [22]	104.4	6.8
	93.4 [22]	102.8	-9.4
	120.5 [22]	122.3	-1.8
	81.4 [22]	84.6	-3.2

Table 1 (Continued)

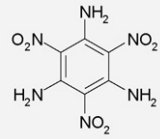
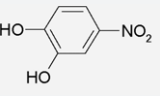
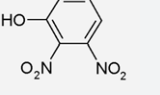
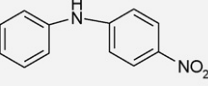
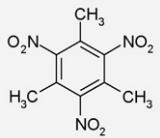
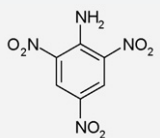
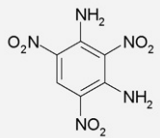
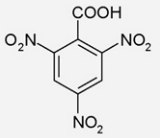
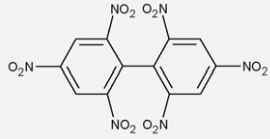
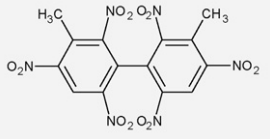
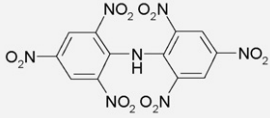
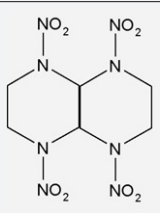
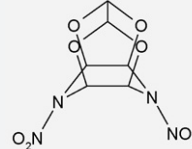
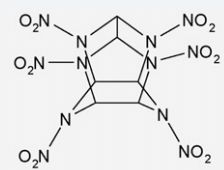
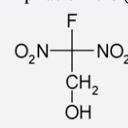
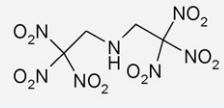
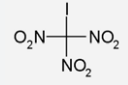
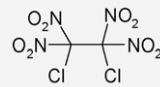
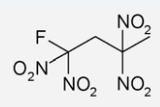
Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
	168.2 [23]	164.5	3.7
	121.1 [22]	123.0	-1.9
	96.6 [22]	102.8	-6.2
	126.2 [22]	110.8	15.4
	103.6 [23]	106.1	-2.5
	125.3 [23]	128.5	-3.2
	140.0 [23]	146.5	-6.5
	154.7 [23]	150.2	4.5
	171.8 [23]	166.8	5.0
	160.8 [23]	174.2	-13.4
	171.6 [23]	170.8	0.8

Table 1 (Continued)

Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
	133.8 [23]	130.3	3.5
	88.3 [22]	86.3	2.0
	98.9 [22]	103.2	-4.3
	83.0 [22]	86.3	-3.3
	173.4 [22]	175.3	-1.9
Cyclic and acyclic nitramines			
	175.3 [23]	174.6	0.7
	52.0 [22]	50.9	1.1
	89.4 [10]	89.7	-0.3
	61.5 [22]	53.3	8.2
	94.2 [22]	93.2	1.0
	106.2 [23]	104.9	1.3
	142.7 [22]	140.9	1.8

Table 1 (Continued)

Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
	154.2 [23]	139.6	14.6
	123.4 [23]	123.6	-0.2
	168.7 [23]	170.5	-1.8
Aliphatic nitro (or nitrate) compounds			
	55.6 [22]	48.1	7.5
	80.8 [22]	98.4	-17.6
	49.0 [22]	47.0	2.0
	88.3 [22]	81.4	6.9
	91.6 [22]	75.2	16.4
Rms deviation (kJ/mol)			6.9

can be used to evaluate their solid phase heats of formation ($\Delta H_f(s)$) [8]:

$$\Delta H_f(s) = \Delta H_f(g) - \Delta H_{sub} \quad (1)$$

There are a variety of approaches for prediction of gas phase heat of formation of energetic compounds [13], in which two simple empirical methods have been recently introduced for selected classes of explosives [14,15]. In contrast, few methods were used to predict heat of sublimation of energetic compounds.

There are several quantum mechanical calculations that can predict the heats of sublimation of energetic compounds. An earlier effort has been introduced by Politzer et al. with a significant success [16]. They used three quantum mechanically parameters: (1) the surface area of the 0.001 electron/bohr³ isosurface of the electron density of the molecule, (2) a measure of the variability of electronic potential on the surface, and (3) the degree of balance between the positive and negative charges on the isosurface. Rice et

al. [11] applied a procedure proposed by Politzer et al. [16] to generate surface electrostatic potentials of individual molecules through using them in empirical equations for heats of sublimation. Byrd and Rice [17] have modified the work of Rice et al. [11] through the incorporation of group additivity and the use of the more complicated 6-311++G(2df,2p) basis set. Hu et al. [18] have also used the empirical relations of Politzer et al. [16] with first-principles density-functional calculations of the electronic properties of the molecular surfaces to predict heats of sublimation of the condensed phases of energetic materials.

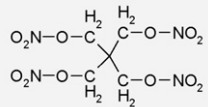
For some classes of energetic compounds, several different approaches have also been introduced. Zeman and Krupka [19] have shown that there are some relationships between heats of sublimation of some polynitro compounds and lattice energies. It was recently indicated that the number of carbon, hydrogen and nitrogen atoms as well as the contribution of some specific groups attached to aromatic ring can be used to predict heats

Table 2

Comparison of calculated heats of sublimation (kJ/mol) of Eq. (3) and quantum mechanical computations of Rice et al. [11] with measured values.

Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (Rice et al. [11])	Dev	ΔH_{sub} (cal)	Dev
Nitroaromatics including polynitro arenes and polynitro heteroarenes					
	103.5 [22]	93.3	10.1	110.5	-7.1
	72.3 [22]	71.5	0.8	90.8	-18.5
	91.2 [22]	98.7	-7.5	90.8	0.4
	92.4 [22]	107.9	-15.6	90.8	1.6
	96.5 [22]	105.9	-9.4	104.5	-8.0
	90.0 [22]	99.6	-9.6	104.5	-14.5
	111.5 [22]	103.8	7.7	114.3	-2.8
	133.1 [22]	112.5	20.6	118.5	14.6
	100.0 [22]	88.7	11.3	102.3	-2.3
Cyclic and acyclic nitramines					
	41.4 [22]	56.1	-14.7	42.7	-1.3
	130.2 [23]	102.5	27.7	130.4	-0.2
	111.0 [22]	88.7	22.3	100.7	10.3
Aliphatic nitro (or nitrate) compounds					
	46.7 [22]	45.2	1.5	47.3	-0.6
	71.0 [22]	82.0	-11.0	87.0	-16.0

Table 2 (Continued)

Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (Rice et al. [11])	Dev	ΔH_{sub} (cal)	Dev
	152.0 [22]	159.8	-7.8	138.0	14.0
rms deviation (kJ/mol)			13.8		9.9

of sublimation of nitroaromatic compounds [9]. The predicted results for 6 nitroaromatics are comparable with complicated quantum mechanical computations of Rice et al. [11]. A simple procedure has also been introduced to predict heats of sublimation of nitramines in which molecular weight and one structural parameter of nitramines would be needed [10]. The rms from experiment for the predicted heats of sublimation of 10 nitramines is 10.10 kJ/mol [10].

The character and intensity of local interactions including magnitude, number, distances and orientation of group dipoles within a molecule are directly connected with the size of a molecule, its conformation, symmetry and with the quantity of the constituents present. The study of heats of sublimation for various polynitro compounds has shown that it is possible to find a general simple correlation on the basis of molecular weight of energetic compounds. Experimental data of 57 nitro compounds including nitroaromatics, cyclic and acyclic nitramines, nitroaliphatics and nitrate esters are given in Table 1. The dependence of their intensity on the magnitude of molecular weight is depicted in Fig. 1. As seen in Fig. 1, enthalpies of sublimation can be related to molecular weights for some nitro compounds. The contribution of some specific polar groups may increase the predicted results on the basis of molecular weight. For some nitro compounds, the reverse situation can be observed for the existence of some structural parameters.

It was found that the molecular weight should be revised for some classes of halogenated nitro compounds because their effects may be different. For nitroaromatics that contain halogens attached to aromatic ring and hydrogen free nitro compounds, deviations

of the predicted heat of sublimation on the basis of molecular weight can be diminished by neglecting atomic weights of halogens. The contribution of atomic weight of halogens should be considered in calculating the molecular weight for the other classes of nitro compounds. To establish a new correlation, various studies of different structural parameters have shown that molecular weight and the contribution of some specific functional groups and structural parameters can be combined by the following general equation with some adjustable coefficients:

$$\Delta H_{sub} = w_1 + w_2 MW' + w_3 C_{In} + w_4 C_{De} \quad (2)$$

where w_1 to w_4 are adjustable parameters; MW' is the molecular weight of nitro compound except halogenated nitroaromatics and hydrogen free nitro compounds for which the revised form should be used, C_{In} is the contribution of specific polar groups attached to aromatic ring, which can increase the predicted results for the presence of some specific polar groups; C_{De} shows the presence of some molecular parameters that may decrease the predicted heats of sublimation.

3. Results and discussion

Experimental data given in Table 1 were used to optimize the values of w_1 to w_4 . Multiple linear regression method [20] was used to find adjustable parameters. The left-division method for solving linear equations uses the least squares method because the equation set is overdetermined [20]. The optimized correlation can be obtained:

$$\Delta H_{sub} = 53.74 + 0.2666 MW' + 13.99 C_{In} - 15.58 C_{De} \quad (3)$$

where ΔH_{sub} is in kJ/mol. As seen in Eq. (3), the coefficients of C_{In} and C_{De} have positive and negative signs, respectively, which are consistent with the role of these structural parameters. We can specify the values of C_{In} and C_{De} according to the following conditions:

3.1. Nitroaromatics

3.1.1. Prediction of C_{In}

We can expect that the existence of some specific polar groups can increase the predicted values of heats of sublimation on the basis of molecular weight.

- (i) The presence of -COOH and -OH functional groups: it was indicated in previous work [9] that the effect of carboxylic acid functional group or two hydroxyl groups under certain conditions on the predicted heats of sublimation is higher than that of other functional groups. This situation can result from the presence of high intermolecular hydrogen bonding. Since intramolecular hydrogen bonding of a group can reduce its ability to form intermolecular hydrogen bonds, it would be expected that the presence of nitro group in ortho-position of -OH can cancel its effect. Thus, $C_{In} = 2.0$ for compounds that have carboxylic acid functional group or two hydroxyl groups. Moreover, for the presence of

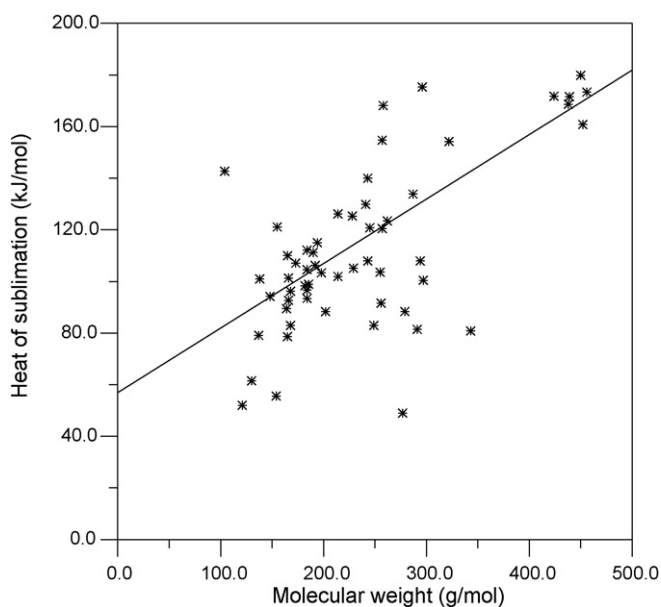


Fig. 1. Experimental heats of sublimation versus molecular weight for different nitroaromatics, nitramines, nitroaliphatics and nitrate esters. The 95% confidence limits for the slope and intercept are 0.286 ± 0.055 and 49.28 ± 13.24 , respectively.

Table 3
Comparison of predicted heats of sublimation (kJ/mol) of further nitroaromatics, nitramines, nitroaliphatics and nitrate esters, which have complex molecular structure, with the experimental data.

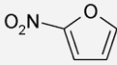
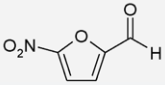
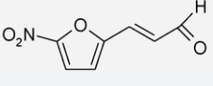
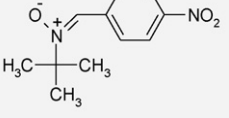
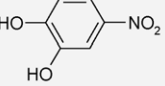
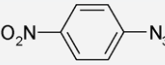
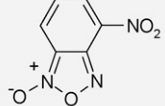
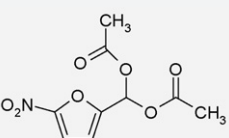
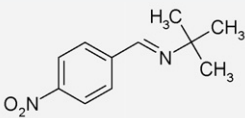
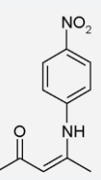
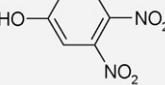
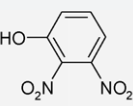
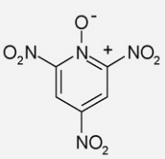
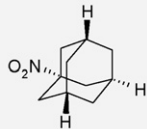
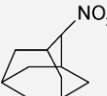
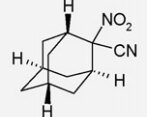
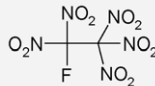
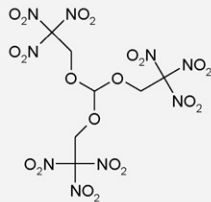
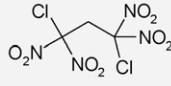
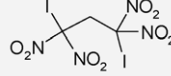
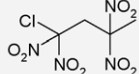
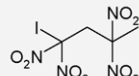
Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
Nitroaromatics including polynitro arenes and polynitro heteroarenes			
	75.3 [22]	83.9	-8.6
	75.3 [22]	91.3	-16.0
	98.0 [22]	98.3	-0.3
	116.5 [22]	112.9	3.6
	121.1 [22]	123.0	-1.9
	81.0 [22]	97.5	-16.5
	97.3 [22]	102.0	-4.7
	126.0 [22]	118.5	7.5
	91.1 [22]	108.7	-17.6
	121.9 [22]	112.4	9.5
	123.5 [22]	102.8	20.7
	96.6 [22]	102.8	-6.2
	106.3 [22]	115.1	-8.8

Table 3 (Continued)

Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
	104.6 [22]	118.8	-14.2
	101.7 [22]	110.8	v9.1
	135.1 [22]	125.7	9.4
	74.5 [22]	95.1	-20.6
	142.7 [22]	137.2	5.5
	151.5 [22]	133.2	18.3
Cyclic and acyclic nitramines			
	142.7 [22]	140.9	1.8
	98.0 [10]	100.9	-2.9
	58.3 [10]	50.1	8.2
	99.2 [22]	93.9	5.3
	81.6 [22]	88.9	-7.3
	104.3 [10]	118.3	-14.0
Aliphatic nitro (or nitrate) compounds			
	84.1 [22]	71.3	12.8

Table 3 (Continued)

Molecular structure	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
	63.6 [22]	55.3	8.3
	58.0 [22]	55.3	2.7
	70.0 [22]	61.9	8.1
	69.0 [22]	74.7	-5.7
	150.0 [22]	154.4	-4.4
	93.7 [22]	85.1	8.6
	111.0 [22]	109.3	1.7
	91.6 [22]	79.6	12.0
	99.2 [22]	104.0	-4.8
Rms deviation (kJ/mol)			10.4

two hydroxyl groups attached to aromatic ring, nitro groups should be separated from -OH at least by one -CH-group, e.g. 4-nitrobenzene-1,2-diol.

- (ii) The presence of amino groups: the introduction of amino groups into a benzene ring having nitro groups is one of the simplest approaches to enhance the thermal stability of explosives [21]. For example, 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) has relatively high heat of sublimation and thermal stability with respect to the other amino derivatives of nitrobenzene. Thus, the value of C_{In} is equal to the number of amino groups in this situation, i.e. $C_n = n_{NH_2}$.

- (iii) The attachment of carbonyl group in form of amide ($Ar-C(=O)N$) or ketone ($Ar-C(=O)R$): carbonyl groups are in resonance with aromatic ring, which can enhance likely to be some coplanar

and rigid. The value of C_{In} here is 0.75 because the contribution of this effect is small.

3.1.2. Prediction of C_{De}

It would be expected that the attachment of alkyl groups, especially bulky group such as tert-butyl, can decrease the intermolecular interactions for high ratio of n_R/n_{NO_2} . For $n_R/n_{NO_2} \geq 1$, the contribution of C_{De} should be considered. If only small alkyl groups such as methyl groups are present, the value of C_{De} equals 1.0. Meanwhile, the values of C_{De} are 2.0 and 3.0 for the existence of one and more than one bulky groups, respectively.

3.2. Nitramines

In crystals of polynitramines, the direct electrostatic interactions are dominant. It was indicated that the number of -CH₂-groups between two nitramine functional groups ($n_{O_2NCH_2NNO_2}$)

in cyclic nitramines is important factor in prediction of heat of sublimation on the basis of molecular weight [10]. The value of $n_{\text{O}_2\text{NNCH}_2\text{NNO}_2}$ has higher contribution in predicting heat of sublimation with respect to MW for cyclic nitramines [10]. For new method, the contributions of C_{In} and C_{De} depend on the number of N–NO₂ groups in cyclic and acyclic nitramines, which are equal to $1.75n_{\text{NNO}_2} - 4$. For five member or higher cyclic nitramines that

have only the fragments $\text{CH}_2\text{—}\overset{\text{NO}_2}{\text{N}}\text{—CH}_2$ and acyclic nitramines, the value of C equals $1.75n_{\text{NNO}_2} - 4$. If the value of C is less than zero, it will be C_{De} . For positive value of C, it is equal to C_{In} .

For nitramines with molecular fragment $\text{NH}=\text{C}=\text{NH}$, the molecular interactions are appreciable so that the value of C_{In} is 4.25. It was shown that this molecular fragment can improve thermodynamic stability of corresponding nitramines [5].

3.3. Nitroaliphatic compounds

For nitroaliphatic compounds, the intermolecular forces are less than the previous categories of energetic compounds. Thus, the predicted heats of sublimation on the basis of molecular weight should be corrected. The value of C_{De} is equal to 3.0 in these compounds.

The values of C_{De} and C_{In} are equal to zero if the conditions to assign different values are not met. R-squared value or the coefficient of determination of this correlation is 0.92 [20] because the presence of a variety of steric, inter- and intramolecular interactions and uncertainty in heats of sublimation data from different sources. Differences of the predictions from the experiments for various methods are given in Table 1. As indicated in Table 1, the rms deviation of the new method from experiment is 6.9 kJ/mol with a maximum deviation of 17.6 kJ/mol. In order to compare the reliability of the present procedure with the quantum mechanical method, the predicted values of heats of sublimation for 15 compounds are given in Table 2. Quantum mechanical computations of Rice et al. [11] are given in Table 2. As shown in Table 2, the rms deviation of this new method (9.9 kJ/mol) is lower than the method of Rice et al. (13.8 kJ/mol) [11]. Thus, the reliability of the present method is higher than quantum mechanical computations of Rice et al. [11]. To test the reliability of the new method, some further energetic compounds with complex molecular structures are also given in Table 3 and the predicted results are compared to the latest experimental data [11]. As seen in Table 3, the rms of different nitro compounds is 10.4 kJ/mol, which is close to the rms deviation values of Tables 1 and 2. The latest reported experimental values of the NIST Chemistry Web Book [22] were taken for comparison in Tables 1–3. The estimated heats of sublimation of 107 different compounds given in Tables 1–3 by new correlation are within ± 21.0 kJ/mol of the measured values.

Theoretical prediction of common and new energetic compounds where experimental data were available, e.g. PETN, TNT, RDX, HMX, TEX, TATB, DATB, tetryl and CL-20, have been given in Tables 1–3. The present method cannot be applied for some energetic compounds that do not contain energetic bonds Ar–NO₂, N–NO₂, C–NO₂ and C–O–NO₂. Thus, heat of sublimation of the other energetic compounds, e.g. AP, lead azide, polynitrogen compounds, etc., with different energetic bonds cannot be calculated by new method.

4. Conclusions

A new general correlation has been developed for simple and reliable prediction of heats of sublimation of nitroaromatics,

nitramines, nitroaliphatics and nitrate esters. The contributions of specific polar groups attached to aromatic ring as well as the presence of some molecular parameters are simple factors, which can increase and decrease the predicted results on the basis of the revised molecular weight. The predicted heats of sublimation by new model give good results with respect to quantum mechanical computations, which are complex and also require special software. The methodology presented here gives the simplest and easiest method and at the same time gives reliable results. This work shows that the accuracy is not necessarily enhanced by greater complexity.

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