Prediction of heats of sublimation of nitroaromatic compounds via their molecular structure

Mohammad Hossein Keshavarz *

Department of Chemistry, Malek-ashtar University of Technology, Shahin-shahr, P.O. Box 83145/115, Islamic Republic of Iran

Abstract

This work presents a new approach to predict heats of sublimation of nitroaromatic compounds derived from their molecular structure information. The number of carbon, hydrogen and nitrogen atoms as well as the contribution of some specific groups attached to aromatic ring would be needed in the new method. Predicted heats of sublimation for 40 nitroaromatic compounds are compared with experimental data. Calculated results for some nitroaromatic compounds are also compared with complicated quantum mechanical computations of Rice et al. [B. M. Rice, S. V. Pai, J. Hare, Combust. Flame 118 (1999) 445] where computed outputs were available. The root mean square deviation (rms) from experiment for the predicted heats of sublimation of 40 compounds by new method is 7.78 kJ/mol with a maximum deviation of 18.52 kJ/mol. The rms deviations of new procedure and reported quantum mechanical method for six nitroaromatic compounds are 9.19 and 10.18 kJ/mol, respectively.
© 2007 Elsevier B.V. All rights reserved.

Keywords: Heats of sublimation; Nitroaromatic compounds; Correlation; Structural parameters

1. Introduction

In an effort to predict various properties of a notional energetic material with the best use of limited resources and to minimize the waste ensuing from experimental measurements, different theoretical approaches have been developed to aid in the formulation of propellants and explosives [1,2]. A long-sought-after goal within the energetic materials community has been to develop capabilities for predicting performance, sensitivity, physical and thermodynamic properties of a new energetic compound before expending resources in its synthesis. Furthermore, different theoretical models can allow experimental researches to expend resources only on those molecules that show promise of enhanced performance, reduced sensitivity or reduced environmental hazard, good physical and thermodynamic properties. For example, sensitivity [3–7], melting point [8,9] and heat of detonation [10–12] of selected class of energetic compounds can be determined by some new methods.

Condensed phase heat of formation is usually the desired quantity for assessment of the energetic material of interest. It can be determined by using the gas phase heat of formation and heat of phase transition (either sublimation or vaporization) according to Hess' law of constant heat summation [13]:

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

$$\Delta H_f(l) = \Delta H_f(g) - \Delta H_{vap} \tag{2}$$

Since condensed phase for most energetic compounds is solid, Eq. (1) can be used to evaluate their solid phase heats of formation. Quantum mechanical computations can be used to predict heats of sublimation of energetic compounds [14–16]. Heat of sublimation is best obtained from solid vapor pressure data by using Clausius-Clapeyron equation [17]. Since the sublimation pressure at the melting point is known with accuracy for only a few cases, it can be calculated from a liquid vapor pressure correlation by extrapolating to melting point [17]. Goodman et al. [18] have recently found that a group-contribution method can be used to estimate heat of sublimation at triple point for organic solids. The purpose of this work is to present a new simple scheme to predict heats of sublimation of nitroaromatic compounds as an important class of energetic compounds. This work assumes that heat of sublimation of a nitoaromatic energetic compound with composition $C_a H_b N_c O_d$ can be determined from the elemental composition

* Tel.: +98 312 522 5071; fax: +98 312 522 5068.
 E-mail addresses: mhkir@yahoo.com, mhkeshavarz@mut-es.ac.ir.

and some structural parameters. The results will be compared with experimental data and some of reported results of complicated quantum mechanical method [15]. It will be shown that results predicted by this simple method are comparable with outputs from complicated quantum mechanical computations and the accuracy is not necessarily enhanced by greater complexity.

2. Theory

2.1. Gas phase heat of formation

To evaluate solid phase heat of formation from Eq. (1) using theoretical prediction alone, different methods can be used. Quantum mechanical and group-contribution methods are two usual procedures for calculating gas phase heats of formation of various compounds. The semi-empirical molecular orbital methods such as PM3, MNDO, MNDO/3, AM1 and molecular mechanics MM2 can be used to estimate gas phase heat of formation for different energetic compounds. For example, Akutsu et al. [19] combined heats of vaporization and sublimation by additivity rule with gas phase heat of formation from PM3 and MM2 to estimate solid and liquid phase heat of formation of nitramines and alkyl nitrate. A group-contribution method, such as Benson, Yoneda and Joback methods, assumes that properties of molecules can be derived from properties of atoms or functional groups from which they are made [17]. Meanwhile, root mean square (rms) deviation of quantum mechanical computations are less than group-contribution methods but they have special complexity and take much time for the optimization of large molecule system. Two new correlations were recently introduced for desk calculations of gas phase heats of formation of selected class of energetic compounds so that they can provide reliable simple pathways as compared to complex quantum mechanical methods [20,21].

2.2. Heat of sublimation

In contrast to the other methods for prediction of gas phase heat of formation, few methods were used to determine heat of sublimation of energetic compounds. Politzer et al. [14] have established that correlations exist between the electrostatic potential of a molecule and heats of sublimation. The predicted heat of sublimation can be represented by:

$$\Delta H_{\text{sub}} = a(\text{SA})^2 + b\sqrt{\sigma_{\text{Tot}}^2 \nu} + c \tag{3}$$

where SA is the surface area of the 0.001 electron/bohr^3 isosurface of the electron density of the molecule, σ_{Tot}^2 is a measure of the variability of electronic potential on the surface and ν is the degree of balance between the positive and negative charges on the isosurface. The constants a, b and c in Eq. (3) are determined from least-squares fitting to experimental values for the heats of sublimation. They applied this procedure to predict heats of sublimation of 34 organic compounds [14]. Rice et al. [15] applied a procedure proposed by Politzer et al. [14] to calculate heats of sublimation of energetic materials. They

used the Gaussian 98 suite of quantum chemistry codes [22] with the 6-31G* basis set [23] and the hybrid B3LYP [24,25] density functional to determine heats of formation and detonation of energetic compounds. Byrd and Rice [16] have also improved an earlier effort of Rice et al. through the use of a larger basis set and the application of group equivalents. They have modified the work of Rice et al. [15] in the prediction of gas, liquid, and solid heat of formation by using quantum mechanical data through the incorporation of group additivity and the use of the more complicated 6-311++G(2df, 2p) basis set. Zeman and Krupka [26] have also found some relationships between heats of sublimation of some polynitro compounds and lattice energies.

3. Results and discussion

Thermo-physical properties of polyfunctional compounds are influenced by different molecular interactions. 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 [27].

The study of heats of sublimation for various nitroaromatic compounds has shown that it is possible to find a new correlation for predicting heats of sublimation. To establish a new correlation, experimental data of various nitroaromatic compounds were taken from literature. For $C_aH_bN_cO_d$ nitroaromatic compounds, it was found that elemental composition and the contribution of some specific groups can influence the values of heats of sublimation. The collected data are listed in Tables 1 and 2

. The study shows that the following general equation with some adjustable coefficients is suitable for this purpose:

$$\Delta H_{\text{sub}} \text{ (kJ/mol)} = x_1 + x_2 a + x_3 b + x_4 c + x_5 C_{\text{SG}} \tag{4}$$

where x_1 to x_5 are adjustable parameters; a, b, c are the number of carbon, hydrogen and nitrogen atoms, respectively; C_{SG} is the contribution of specific polar groups attached to aromatic ring. Experimental data given in Table 1 were used to optimize the values of x_1–x_5. Multiple linear regression method [28] 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 [28]. The results give the following optimized correlation:

$$\Delta H_{\text{sub}} \text{ (kJ/mol)} = 64.51 + 4.555a - 2.763b$$
$$+ 10.32c + 16.51 C_{\text{SG}} \tag{5}$$

Different values of C_{SG} for various polar groups attached to nitroaromatic ring were studied and optimized with experimental data. As seen in Eq. (5), coefficient of C_{SG} has a positive sign. This confirms that the existence of some specific polar groups can influence the values of heat of sublimation. Moreover, it was found that the effects of carboxylic acid functional group or two hydroxyl groups on predicted heats of sublimation are higher than the other specific groups. The value of C_{SG} can be determined as follows:

Table 1
Comparison of predicted heats of sublimation (kJ/mol) of nitroaromatic compounds with the experimental data

Name	Molecular structure	Molecular formula	C_{SG}	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
1-Methy-4-nitrobenzene		$C_7H_7NO_2$	0	79.1 [27]	87.37	−8.27
4-Nitroaniline		$C_6H_6N_2O_2$	0	100.9 [27]	95.89	5.01
1-Methyl-2,4-dinitrobenzene		$C_7H_6N_2O_4$	0	100 [27]	100.44	−0.44
1-Nitronaphthalene		$C_{10}H_7NO_2$	0	107.1 [27]	101.03	6.07
2-Methyl-1,3,5-trinitrobenzene		$C_7H_5N_3O_6$	0	104.6 [27]	113.52	−8.92
				118.4 [28]		4.88
2-Methyl-1,3-dinitrobenzene		$C_7H_6N_2O_4$	0	98.3 [27]	100.44	−2.14
1,4-Dinitrobenzene		$C_6H_4N_2O_4$	0	96.2 [27]	101.42	−5.22
2,4-Dinitrophenol		$C_6H_4N_2O_5$	0	104.6 [27]	101.42	3.18
2,4,6-Trinitrophenol		$C_6H_3N_3O_7$	0	105.1 [27]	114.49	−9.39
1,2-Dinitrobenzene		$C_6H_4N_2O_4$	0	82.9 [27]	101.42	−18.52
2,4,6-Trimethylnitrobenzene		$C_9H_{11}NO_2$	0	78.6 [27]	85.42	−6.82
2-Methyl-4,6-dinitrophenol		$C_7H_5N_2O_5$	0	103.3 [27]	100.44	2.86
2-Nitrodiphenylamine		$C_{12}H_{10}N_2O_2$	0	101.9 [27]	112.17	−10.27
N,N-Dimethyl-4-nitroaniline		$C_8H_{10}N_2O_2$	0	101.3 [27]	93.95	7.35
2,4,6-Trinitro-1,3-benzenediol		$C_6H_3N_3O_8$	0	120.8 [27]	114.49	6.31

Table 1 (*Continued*)

Name	Molecular structure	Molecular formula	C_{SG}	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
3-Nitroacetophenone		$C_8H_7NO_3$	0.75	110 [27]	104.30	5.70
2,6-Dinitrophenol		$C_6H_4N_2O_5$	0	112.1 [27]	101.42	10.68
N,N-Dimethyl-3-nitroaniline		$C_8H_{10}N_2O_2$	0	92.7 [27]	93.95	−1.25
1,3,5-Trinitro-2,4-dimethyl-5-tert-butylbenzene		$C_{12}H_{15}N_3O_6$	0	100.4 [27]	108.67	−8.27
2-Methoxy-1,3,5-trinitrobenzene		$C_7H_5N_3O_7$	1	133.1 [27]	130.03	3.07
4-*tert*-Butyl-3,5-dinitro-2,6-dimethylacetophenone		$C_{14}H_{18}N_2O_5$	0.75	107.9 [27]	111.55	−3.65
2,4-Dimethyl-1,3,5-trinitrobenzene		$C_8H_7N_3O_6$	0	129.8 [27,28]	112.55	17.25
3-Methyl-2,4,6-trinitrophenol		$C_7H_5N_3O_7$	0	104.6 [27]	113.52	−8.92
				111.2 [28]		−2.32
N,N-Dimethyl-4-nitrobenzamide		$C_9H_{10}N_2O_3$	0.75	115 [27]	110.88	4.12
1,1'-(1,2-ethenediyl)bis[2,4,6-trinitrobenzene]		$C_{14}H_6N_6O_{12}$	0	179.9 [27]	173.59	6.31
8-Hydroxy-5-nitroquinoline		$C_9H_6N_2O_3$	0	111.2 [27]	109.55	1.65
2,5-Dinitrophenol		$C_6H_4N_2O_5$	0	93.4 [27]	101.42	−8.02
2-Ethoxy-1,3,5-trinitrobenzene		$C_8H_7N_3O_7$	1	120.5 [27]	129.06	−8.56

Table 1 (*Continued*)
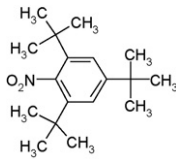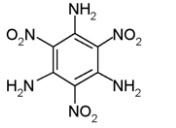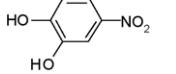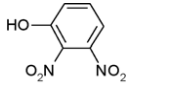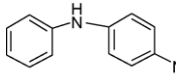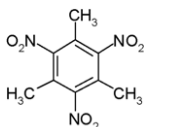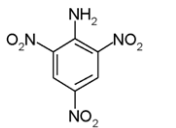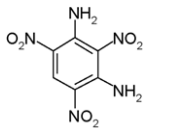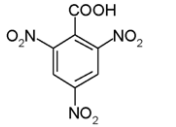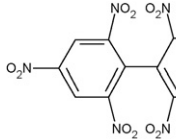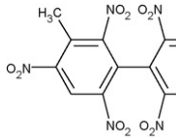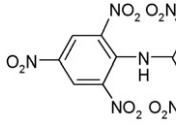
Name	Molecular structure	Molecular formula	C_{SG}	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev
2,4,6-Tri-*tert*-butylnitrobenzene		$C_{18}H_{29}NO_2$	0	81.4 [27]	76.68	4.72
2,4,6-Triamin-1,3,5-trintrobenzene		$C_6H_6N_3O_6$	2	168.2 [27]	170.16	−1.96
4-Nitro-1,2-benzenediol		$C_6H_4N_2O_5$	2	121.1 [27]	121.35	−0.25
2,3-Dinitrophenol		$C_6H_4N_2O_5$	0	96.6 [27]	101.42	−4.82
4-Nitrodiphenylamine		$C_{12}H_{10}N_2O_2$	0	126.2 [27]	112.17	14.03
2,4,6-Trimethyl-1,3,5-trinitrobenzene		$C_9H_9N_3O_6$	0	103.6 [27]	111.58	−7.98
1-Amino-2,4,6-trinitrobenzene		$C_6H_4N_4O_6$	0	125.3 [28]	122.05	3.25
1,3-Diamino-2,4,6-trinitrobenzene		$C_6H_5N_5O_6$	0	140 [28]	129.60	10.40
2,4,6-Trinitrobenzoic acid		$C_7H_3N_3O_8$	2	154.7 [28]	152.06	2.64
1,3,5-Trinitro-2-(2,4,6-trinitrophenyl)-benzene		$C_{12}H_4N_6O_{12}$	0	171.8 [28]	170.01	1.79
1,3,5-Trinitro-6-methyl-2-(2,4,6-trinitro-3-methylphenyl)-benzene		$C_{14}H_8N_6O_{12}$	0	160.8 [28]	168.06	−7.26
2,4,6-Trinitro-*N*-(2,4,6-trinitrophenyl)-aniline		$C_{12}H_5N_7O_{12}$	0	171.6 [28]	177.56	−5.96
rms deviation (kJ/mol)						7.78

Table 2
Comparison of calculated heats of formation of Eq. (5) and quantum mechanical computations of Rice et al. [15] with measured values

Name	Molecular structure	Molecular formula	C_{SG}	ΔH_{sub} (exp)	ΔH_{sub} (cal)	Dev	ΔH_{sub} (Rice et al.)	Dev
4-Nitrophenol		$C_6H_5NO_3$	0	92.39 [27]	88.34	4.05	107.95	−15.56
2-Nitrophenol		$C_6H_5NO_3$	0	72.3 [27]	88.34	−16.04	71.55	0.75
3-Nitroaniline		$C_6H_6N_2O_2$	0	96.5 [27]	95.89	0.61	105.86	−9.36
1,3,5-Trinitrobenzene		$C_6H_3N_3O_6$	0	99.6 [27]	114.49	−14.89	93.30	6.30
				107.3 [28]		−7.19	93.30	14.00
3-Nitrophenol		$C_6H_5NO_3$	0	91.23 [27]	88.34	2.89	98.74	−7.51
2-Nitroaniline		$C_6H_6N_2O_2$	0	90 [27]	95.89	−5.89	99.58	−9.58
rms deviation (kJ/mol)						9.19		10.18

All data are in kJ/mol.

(a) $C_{SG} = 1.0$ for alkoxy (−OR) attached to nitroaromatic ring, e.g. 2-methoxy-1,3,5-trinitrobenzene.
(b) $C_{SG} = 0.75$ for nitroaromatic compounds which contain carbonyl in form of −C(=O)NRR' or −C(=O)–R, where R and R' are alkyl groups, attached to aromatic ring, e.g. 3-nitroacetophenone.
(c) $C_{SG} = 2.0$ for compounds that have carboxylic acid functional group or two hydroxyl groups or three amino groups. In the second situation, nitro groups should be separated from −OH at least by one −CH− group, e.g. 4-nitrobenzene-1,2-diol.

As seen in Table 1, heats of sublimation of 40 different nitroaromatic compounds were calculated and compared with the experimental values. To test the validity of the correlation with respect to quantum mechanical computations of Rice et al. [15] where computed outputs were available, heats of sublimation of six aromatic energetic compounds (corresponding to seven measured values) are calculated and compared with quantum mechanical computations, which are given in Table 2. Differences of the predictions from the experiments for various methods are given in Tables 1 and 2. As indicated in Table 1, the root mean square deviation of the new method from experiment is 7.78 kJ/mol with a maximum deviation of 18.52 kJ/mol. As seen in Table 2, the rms of Eq. (5) is 9.19 kJ/mol which is surprisingly smaller than the rms deviation value 10.18 kJ/mol for computed values of Rice et al. [15]. Due to the existence of the variety of steric, inter- and intramolecular interactions and uncertainty in heats of sublimation data

from different sources, e.g. 104.6 [29] and 111.2 kJ/mol [30] for 3-methyl-2,4,6-trinitrophenol, R-squared value or the coefficient of determination of this correlation is 0.92 [28]. Since data from the NIST Chemistry Web Book [29] may contain different reported values from different sources, e.g. 100.2 and 91.23 kJ/mol are two different reported experimental data for 3-nitrophenol, the latest reported experimental values of this reference were taken for comparison with the mentioned method.

As indicated in Tables 1 and 2, the estimated heats of sublimation of nitroaromatic compounds by new correlation are within ±10.0 kJ/mol of 42 measured values and more than ±10.0 kJ/mol for remainder nine experimental data (corresponding to 46 molecules). Eq. (5) gives the same prediction for different isomers because deviations of heats of sublimation for different isomers are usually small. For example, three isomers 2,3-dinitrophenol, 2,4-dinitrophenol and 2,6-dinitrophenol have experimental heats of sublimation 96.6, 104.6 and 112.1 kJ/mol [29], respectively. Calculated heat of sublimation for these isomers is 101.42 kJ/mol which is close to measured values.

Visual comparisons of the predictions with experimental data are also given in Figs. 1 and 2. Fig. 1 provides the comparison between measured data and predictions of new method. Fig. 2 shows a comparison between calculated values of Eq. (5) and computed results of Rice et al. [15] with experimental values. In each of these figures, exact agreement between the experiment and predicted values is presented by the line that bisects each figure along the diagonal. As evident in Figs. 1 and 2, the new method shows good agreement with experimental data. How-
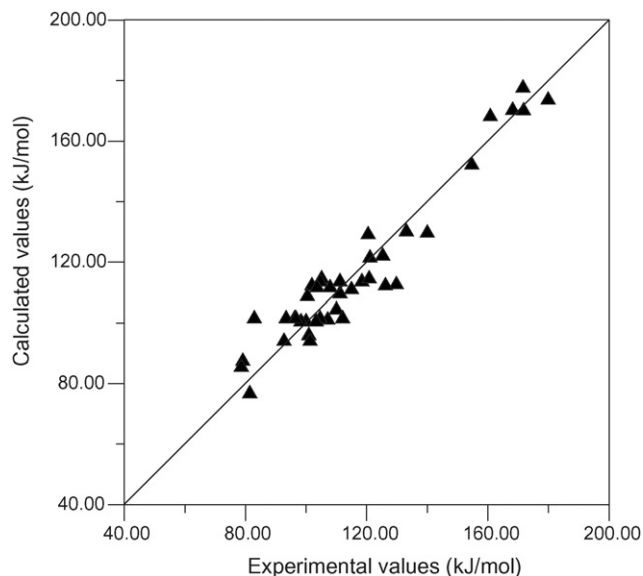
Fig. 1. Calculated heats of sublimation vs. experimental data for $C_aH_bN_cO_d$ nitroaromatic compounds. The solid lines represent exact agreement between predictions and experiment. Filled triangles denote calculated results of new method.
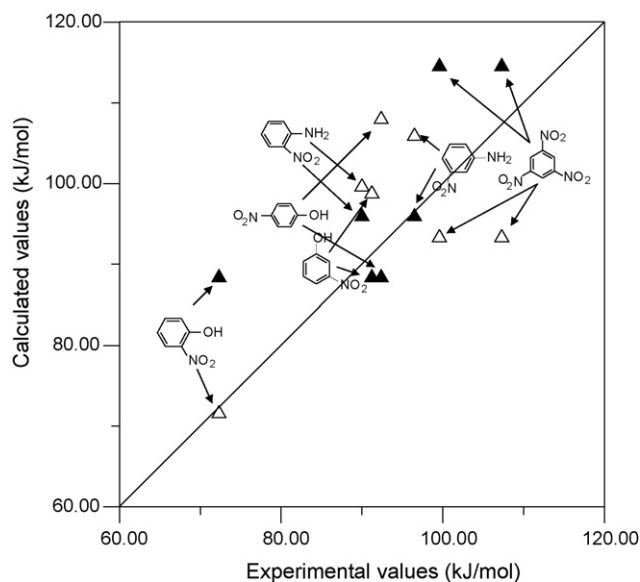

Fig. 2. Calculated heats of sublimation vs. experimental data for $C_aH_bN_cO_d$ nitroaromatic compounds. The solid lines represent exact agreement between predictions and experiment. Filled and hollow triangles denote calculated results of new method and Rice et al. [15]. Molecular structures of nitroaromatic compounds have also been inserted.

ever, this may be taken as appropriate validation test of the new method for nitroaromatic compounds.

4. Conclusions

Reliable predictions of various aspects of energetic compounds are a continuing need in the field of energetic materials. In this paper, a simple approach is introduced for calculating heats of sublimation of nitroaromatic energetic compounds without the need of any experimental data of the new substance. The methodology presented here is much simple for rapid desk calculation of heats of sublimation with about the same reliance on their answers as one could expect from complex quantum mechanical computer programs. However, the estimated heats of sublimation can be used easily with various methods for calculating gas phase heats of formation to predict solid phase heats of formation of nitroaromatic compounds.

Acknowledgement

References

[1] A.K. Sikder, G. Maddala, J.P. Agrawal, H. Singh, Important aspects of behaviour of organic energetic compounds: a review, J. Hazard. Mater. A 84 (2001) 1–26.

[2] M.H. Keshavarz, A simple theoretical prediction of detonation velocities of non-ideal explosives only from elemental composition, in: P.B. Warey (Ed.), New Research on Hazardous Materials, Nova Science Publishers, Inc., 2006 (Chapter 8).

[3] M.H. Keshavarz, H.R. Pouretedal, Simple empirical method for prediction of impact sensitivity of selected class of explosives, J. Hazard. Mater. A 124 (2005) 27–33.

[4] M.H. Keshavarz, M. Jaafari, Propellants, investigation of the various structure parameters for predicting impact sensitivity of energetic molecules via artificial neural network, Explos. Pyrotechn. 31 (2006) 216–225.

[5] M.H. Keshavarz, H.R. Pouretedal, A. Semnani, Novel correlation for predicting impact sensitivity of nitroheterocyclic energetic molecules, J. Hazard. Mater. A 141 (2007) 803–807.

[6] M.H. Keshavarz, H. Motamedoshariati, H.R. Pouretedal, M. Kavosh Tehrani, A. Semnani, Prediction of shock sensitivity of explosives based on small scale gap test, J. Hazard. Mat. A 145 (2007) 109–112.

[7] M.H. Keshavarz, Prediction of impact sensitivity of nitroaliphatic, nitroaliphatic containing other functional groups and nitrate explosives, J. Hazard. Mater. A 148 (2007) 648–652.

[8] M.H. Keshavarz, Approximate prediction of melting point of nitramines, nitrate esters, nitrate salts and nitroaliphatics energetic compounds, J. Hazard. Mater. A 138 (2006) 448–451.

[9] M.H. Keshavarz, H.R. Pouretedal, New approach for predicting melting point of carbocyclic nitroaromatic compounds, J. Hazard. Mater. A 148 (2007) 592–598.

[10] M.H. Keshavarz, H.R. Pouretedal, An empirical method for predicting detonation pressure of CHNOFCl explosives, Thermochim. Acta 414 (2004) 203–208.

[11] M.H. Keshavarz, Simple procedure for determining heats of detonation, Thermochim. Acta 428 (2005) 95–99.

[12] M.H. Keshavarz, Determining heats of detonation of non-aromatic energetic compounds without considering their heats of formation, J. Hazard. Mater. A 142 (2007) 54–57.

[13] P.W. Atkins, Physical Chemistry, Oxford University Press, Oxford, 1982.

[14] P. Politzer, J.S. Murray, M.E. Grice, M. DeSalvo, E. Miller, Calculation of heats of sublimation and solid phase heats of formation, Mol. Phys. 91 (1997) 923–928.

[15] B.M. Rice, S.V. Pai, J. Hare, Predicting heats of formation of energetic materials using quantum mechanical calculations, Combust. Flame 118 (1999) 445–458.

[16] E.F.C. Byrd, B.M. Rice, Improved prediction of heats of formation of energetic materials using quantum mechanical calculations, J. Phys. Chem. A 110 (2006) 1005–1013.

[17] R.C. Reid, J.M. Prausnitz, B.E. Poling, The Properties of Gases and Liquids, 4th ed., McGraw-Hill, New York, 1987.

[18] B.T. Goodman, W.V. Wilding, J.L. Oscarson, R.L. Rowley, Use of the DIPPR database for the development of QSPR correlations: solid vapor

pressure and heat of sublimation of organic compounds: proceedings of the fifteenth symposium on thermophysical properties, part I, Int. J. Thermophys. 25 (2004) 337–350.

[19] Y. Akutsu, R. Che, M. Tamura, Calculations of heats of formation for nitramines and alkyl nitrates with PM3 and Mm2, J. Energetic Mater. 11 (3) (1993) 195–203.

[20] M.H. Keshavarz, M. Kavosh Tehrani, H.R. Pouretedal, A. Semnani, A new pathway for quick estimation of gas phase heat of formation of non-aromatic energetic compounds, Indian J. Eng. Mater. Sci. 13 (2006) 542–548.

[21] M.H. Keshavarz, M. Kavosh Tehrani, A new method for determining gas phase heats of formation of aromatic energetic compounds, Propellants Explos. Pyrotechn. 32 (2007) 155–159.

[22] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, V.G. Zakrzewski, J.A. Montgomery, R.E. Statmann, J.C. Burant, S. Dapprich, J.M. Millam, A.D. Daniels, K.N. Kudin, M.C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G.A. Petersson, P.Y. Ayala, Q. Cui, K. Morokuma, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J. Cioslowski, J.V. Oritz, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P.M.W. Gill, B.G. Johnson, W. Chen, M.W. Wong, J.L. Andrs, M. Head-Gordon, E.S. Replogle, J.A. Pople, Gaussian 98, Gaussian Inc., Pittsburgh, PA, 1998.

[23] W.J. Hehre, L. Rdom, P.V.R. Schleyer, J.A. Pople, Ab Initio Molecular Orbital Theory, Wiley, New York, 1986, p. 271, 298.

[24] A.D. Becke, Density-functional thermochemistry. III. The role of exact exchange, J. Chem. Phys. 98 (1993) 5648–5652.

[25] C. Lee, W. Yang, R.G. Parr, Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density, Phys. Rev. B 37 (1998) 785–789.

[26] S. Zeman, M. Krupka, Some predictions of the heats of fusion, heats of sublimation and lattice energies of energetic materials, HanNeng CaiLiao 10 (2002) 27–33.

[27] A. Bondi, Physical Properties of Molecular Crystals, in: Liquids and Glasses, Wiley, London, 1968.

[28] W.J. Palm III, Matlab for Engineering Applications, WBC/McGraw-Hill, 1999, p. 334.

[29] NIST Standard Reference Data Base Number 69, which can be accessed electronically through the NIST Chemistry Web Book (http://webbook.nist.gov/chemistry/); references for individual molecules are given therein.

[30] S. Zeman, M. Krupka, New aspects of impact reactivity of polynitro compounds. Part III. Impact sensitivity as a function of the intermolecular interactions, Propellants Explos. Pyrotechn. 28 (2003) 301–307.