

A New Computer Code for Prediction of Enthalpy of Fusion and Melting Point of Energetic Materials

Mohammad Hossein Keshavarz*[a]

Abstract: The prediction of phase change properties of energetic materials is important for the assessment of hazardous energetic materials. A novel user-friendly computer code, written in Visual Basic, is introduced to predict the melting point and the enthalpy of fusion of energetic materials by only using their molecular structure parameters. It can be used for different types of energetic compounds including polynitro arenes, polynitro heteroarenes, acyclic

and cyclic nitramines, nitrate esters, and nitroaliphatic. The predicted results were compared with several of the best available methods, which confirmed the higher reliability of the new computer code for some new and well-known energetic compounds with complex molecular structures. This code can be used for designing of energetic compounds with desirable phase change properties.

Keywords: Energetic material • Melting point • Enthalpy of fusion • Computer code

1 Introduction

Energetic materials contain metastable molecules, for many of which the experimental thermophysical property data have not been published yet. Due to their expensive and often hazardous synthesis, testing, and fielding, elimination of a poor candidate before investing in synthesis and testing is of great value. Furthermore, the safety for the scientists and engineers who work with them should be considered. The relationship between the molecular structures of energetic compounds and their various properties such as performance, sensitivity, physical and thermodynamic properties is very important [1–3].

The detonation performance of the energetic compounds under consideration can be calculated by complex well-known thermochemical/hydrodynamic computer codes such as CHEETAH [4] through appropriate equations of state. LOTUSES [5] and EDPHT [6–8] are two simple computer codes that are based on empirical models. It should be mentioned that LOTUSES [5] can be used to predict the gas phase enthalpy of formation, heat of explosion, volume of explosion, gaseous products, and other related performance parameters. EDPHT [6–8] was designed to evaluate various detonation parameters and sensitivity including crystal density, condensed phase heat of formation, activation energy of thermolysis, the velocity of detonation, detonation pressure, heat of detonation, detonation temperature, Gurney velocity, adiabatic exponent and specific impulse as well as electrostatic, impact and shock sensitivities of high explosives.

The purpose of this work is to develop a novel computer code for the prediction of melting point and enthalpy of fusion of various classes of energetic compounds on the basis of recent developments of the predictive methods.

This computer code is able to calculate melting point and enthalpy of fusion of different types of energetic compounds including polynitro arene, polynitro heteroarene, acyclic and cyclic nitramine, nitrate ester, and nitroaliphatic compounds. For some newly reported energetic compounds, this code is also tested.

2 Theory

Some approaches for the calculation of melting point and enthalpy of fusion of energetic compounds were developed. Special attention has been paid on the evaluation of melting point because large numbers of experimental data exist for melting points of different classes of energetic compounds. For the new computer code it is important to use methods, which are applicable for a wide range of different classes of energetic compounds. Molecular dynamics [9], quantitative structure-property/activity relationships (QSPR/QSAR) [10], group additivity [11], and simple approaches [12–21] have been recently introduced to predict melting points and enthalpies of fusion.

Molecular dynamics are able to predict melting points of energetic compounds through simulation of solid to liquid phase transitions [9]. This approach is complex and difficult

[a] M. H. Keshavarz
Department of Chemistry
Malek-ashtar University of Technology
Shahin-shahr P. O. Box 83145/115, Iran
*e-mail: mhkeshavarz@mut-es.ac.ir
keshavarz7@gmail.com

because the presence of free energy barrier for the formation of a liquid-solid interface, which can cause superheating in a perfect crystal.

QSPR/QSAR can be used to predict physicochemical parameters based on the structure of an organic compound. They connect physical or chemical properties to a set of molecular descriptors, which have developed relationships for use in different fields [10]. Different molecular descriptors such as constitutional, geometric, electrostatic, or quantum-chemical may be used [10]. However, the main aim of QSPR/QSARs is the identification of the appropriate set of descriptors that allow the desired attribute of the compound to be adequately predicted. These methods have a key limitation because the set of organic compounds used to develop the relationship should be similar to those compounds, for which predictions are desired.

Group additivity approaches [11] can be used to estimate melting point and enthalpy of fusion of a compound by summing the number frequency of each group multiplied by its contribution. For prediction of melting points of pure compounds, the Joback-Reid (JR) [22] method is popular among the other group-contribution methods, which can be given as:

$$T_m [\text{K}] = 122.5 + \sum n_i GC_i \quad (1)$$

where n_i is the number of groups of type i and GC_i is the group contributions of the melting points resulting from the group i of the molecule. For different classes of energetic compounds, the predicted results using group additivity approaches may give large deviations [2].

For simple organic molecules and/or homologous series, suitable models have been developed. Jain and co-workers [23] applied a combined approach of group contribution and non-additive molecular parameters to predict the melting points of aliphatic compounds and more complex organic molecules. Simamora and Yalkowsky [24] have also used rotational symmetry as a non-additive non-constitutive property to get a more accurate estimation of melting points of organic aromatics and heterocycles with respect to the JR method [22].

For predicting the enthalpy of fusion by group additivity approaches, each molecule can be broken down into defined groups and for each group a standard enthalpy value can be assigned. However, the calculated enthalpy of fusion can be given as:

$$\Delta H_{\text{fus}} = \sum n_i (\Delta H_{\text{fus}})_i \quad (2)$$

where $(\Delta H_{\text{fus}})_i$ is the contribution of the group i to the enthalpy of fusion. Some investigations have been made to use Equation (2) for different types of organic compounds [23]. For some organic energetic compounds, group contribution approaches yield large deviations in the predicted

values of enthalpy of fusion [13,15,18,19,21]. Thus, one may use group contribution methods for a very approximate guess of both melting point and the enthalpy of fusion of energetic compounds.

For some classes of energetic compounds, simple correlations have been recently introduced to predict their melting points and enthalpies of fusion [12–21]. It is important to select a suitable prediction model that can be applied for large classes of energetic compounds because the presence of impurity or thermal instability of energetic compounds may thwart the experimental data of melting point. Among these relationships, two suitable correlations have been developed that can be applied for large classes of energetic compounds including at least one of the groups Ar–NO₂, C–NO₂, C–ONO₂ or N–NO₂ [20,21].

Although group additivity approaches have the advantages of quick estimates but many of them are of questionable accuracy and unknown reliability.

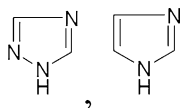
2.1 Melting Point

For various aromatic and non-aromatic energetic compounds containing Ar–NO₂, C–NO₂, C–ONO₂, or N–NO₂ groups, suitable combination of elemental composition and the presence of some structural parameters can be used to predict melting point as:

$$T_m [\text{K}] = 326.9 + 5.524a + 2.646b + 14.60c - 2.130d + 101.2T_{\text{In,m}} - 68.08T_{\text{De,m}} \quad (3)$$

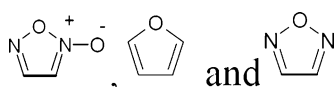
where a , b , c and d are the number of carbon, hydrogen, oxygen, and nitrogen atoms, respectively; $T_{\text{In,m}}$ and $T_{\text{De,m}}$ represent the positive and negative non-additive contributions of some structural parameters. The correcting functions $T_{\text{In,m}}$ and $T_{\text{De,m}}$ are defined as follows:

- Presence of an amino (–NH₂) group: (i) The number of amino groups per cycle of aromatic ring in polynitro arenes or non-aromatic energetic compounds: The values of $T_{\text{In,m}}$ equal 0.5 and 2.0 for the existence of one and higher number of amino groups, respectively, except o-nitroaniline because intramolecular hydrogen bonding may cancel the effect of amino group. (ii) Polynitro heteroarenes: The value $T_{\text{In,m}}$ equals 1.0 for the attachment of amino groups to heterocyclic aromatic compounds.
- Existence of some specific polar groups and molecular fragments: (i) Nitroaromatics: The value of $T_{\text{In,m}}$ equals to 0.75 for the attachment of –COOH, –NH–CO–, and at least two –OH groups to aromatic ring. For the existence of –NO₂, R₂N– and –N–C(=O)– in *para* position of the nitro group, $T_{\text{In,m}}$ equals to 0.75. The value of $T_{\text{In,m}}$ equals to 1.0 for the presence of –C=C–Ar. (ii) Non-aromatic energetic compounds: The value of $T_{\text{In,m}}$ is 1.0 for the existence of some specific polar



groups such as $-\text{NH}-\text{NO}_2$, NH_4^+ , and more than one $-\text{OH}$ as well as one cyclic ether or carbocyclic cage energetic compounds.

- (c) Alkyl- or alkoxy-substituted nitroaromatics: The values of $T_{\text{De,m}}$ are 1.0 and 0.5 for the ratios $n(\text{NO}_2)/n(\text{R,OR}) \leq 1$ and $n(\text{NO}_2)/n(\text{R,OR}) > 1$, respectively.
- (d) Alkyl nitramine groups attached to aromatic rings: The value of $T_{\text{De,m}}$ can be found from $T_{\text{De,m}} = 0.7 \times$ the number of alkyl nitramine groups.
- (e) Specific structural factors: The value of $T_{\text{De,m}}$ equals to 1.0 for the existence of



- (f) Mononitro-substituted aromatic compounds: The value of $T_{\text{De,m}}$ is equal to 1.0.
- (g) Non-aromatic energetic compounds with general formula $-\text{CH}-(\text{NO}_2 \text{ or } \text{ONO}_2)_n$: The values of $T_{\text{De,m}}$ depend on the number of nitro and nitrate groups: (i) If $n = 1$, then $T_{\text{De,m}} = 2.0$; (ii) If $n = 2$ or 3, then $T_{\text{De,m}} = 1.0$.
- (h) Polycyclic nitroaromatic compounds: The ratio of the number of nitro groups $n(\text{NO}_2)$ to the number of aromatic rings $n(\text{aromatic ring})$ is important in these compounds. If $n(\text{NO}_2)/n(\text{aromatic ring}) > 2.5$ then $T_{\text{In,m}} = 2.0$ for the existence of three aromatic rings. Meanwhile, for the presence of four member rings, if $n(\text{NO}_2)/n(\text{aromatic ring}) > 2.5$ then $T_{\text{De,m}} = 1.0$.
- (i) Cyclic nitramines containing methylene units: The ratio of the number of nitramine groups $n(\text{NNO}_2)$ to the number of methylene units $n(\text{CH}_2)$ is important here: (i) If the ratio $n(\text{NNO}_2)/n(\text{CH}_2) \geq 1.0$, then $T_{\text{In,m}} = 0.5$; (ii) If the ratio $n(\text{NNO}_2)/n(\text{CH}_2) \leq 0.2$, then $T_{\text{De,m}} = 1.2$.

The values of $T_{\text{In,m}}$ and $T_{\text{De,m}}$ are equal to zero for the other ratios of $n(\text{NO}_2)/n(\text{aromatic ring})$ and $n(\text{NNO}_2)/n(\text{CH}_2)$ except mentioned above.

2.2 Enthalpy of Fusion

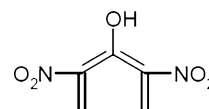
For energetic compounds with general formula $\text{C}_a\text{H}_b\text{N}_c(\text{O or S})_d(\text{halogen})_e$, the following correlation can be used to predict enthalpy of fusion:

$$\Delta H_{\text{fus}} [\text{kJ mol}^{-1}] = 0.542a + 1.490b + 2.044c + 1.252d + 1.839e + 9.848\Delta H_{\text{Inc,fus}} - 11.68\Delta H_{\text{Dec,fus}} \quad (4)$$

where $\Delta H_{\text{Inc,fus}}$ and $\Delta H_{\text{Dec,fus}}$ denote increasing and decreasing

effects of correcting functions, which are demonstrated as follows:

- (a) Effects of $-\text{OH}$ and $-\text{COOH}$ groups: The value of $\Delta H_{\text{Inc,fus}}$ equals to 0.4 for the presence of these groups except mono hydroxyl group between two nitro groups or *ortho* to alkyl group in which the value of $\Delta H_{\text{Inc,fus}} = 0.0$.



- (b) Influence of $-\text{NH}_2$ groups: For the presence of one or two $-\text{NH}_2$ groups, the value of $\Delta H_{\text{Inc,fus}}$ equals to 0.7 except if there is amino group in *ortho* position of nitro groups for mononitro derivatives in which $\Delta H_{\text{Inc,fus}} = 0.0$. The value of $\Delta H_{\text{Inc,fus}}$ is 2.6 for the presence of more than two amino groups attached to aromatic ring.
- (c) Number of $-\text{NNO}_2$ groups in acyclic nitramines $n_{\text{NNO}_2}^{\text{acycl}}$: For the existence of more than three nitramine groups, $\Delta H_{\text{Inc,fus}} = n_{\text{NNO}_2}^{\text{acycl}} - 2$.
- (d) Disubstituted nitroaromatics: The value of $\Delta H_{\text{Inc,fus}}$ equals 1.1 for dinitronaphtalene and the existence of polar groups such as $-\text{OH}$ and $-\text{NO}_2$ *para* to nitro groups in disubstituted benzene derivatives.
- (e) Nitroaromatics containing more than one benzene ring: The value of $\Delta H_{\text{Dec,fus}}$ equals to 0.5 except for the presence of sulfur between two benzene rings.
- (f) Cyclic nitramines with more than six member ring containing only carbon and nitrogen atoms ($m_{\text{cyc}}^{>6}$): The value of $\Delta H_{\text{Dec,fus}}$ is equal to $(m_{\text{cyc}}^{>6} - 6)/4 + 0.5$.
- (g) Nonaromatics containing $-\text{NO}_2$ and $-\text{ONO}_2$ groups: The values of $\Delta H_{\text{Dec,fus}}$ and $\Delta H_{\text{Inc,fus}}$ equal to 0.4 and 1.1 for less than or equal to three and higher than three $-\text{NO}_2$ (or $-\text{ONO}_2$) groups, respectively.

The correcting functions $T_{\text{De,m}}$ and $T_{\text{In,m}}$ as well as $\Delta H_{\text{Inc,fus}}$ and $\Delta H_{\text{Dec,fus}}$ in Equation (3) and Equation (4) are equal to zero if the conditions for giving them various values are not met.

3 Computation of Melting Point and Enthalpy of Fusion by the New Computer Code

The new version of the computer code EDPHT 4.0 is able to calculate melting point and enthalpy of fusion beside performance, density, heat of formation and sensitivity. It is improved to run on windows operating system using modern modular and object-oriented techniques in Visual Basic 6.0. It occupies about 5.0 MB of hard disk space in the computer. It can be installed in Windows 98, 2000, XP as

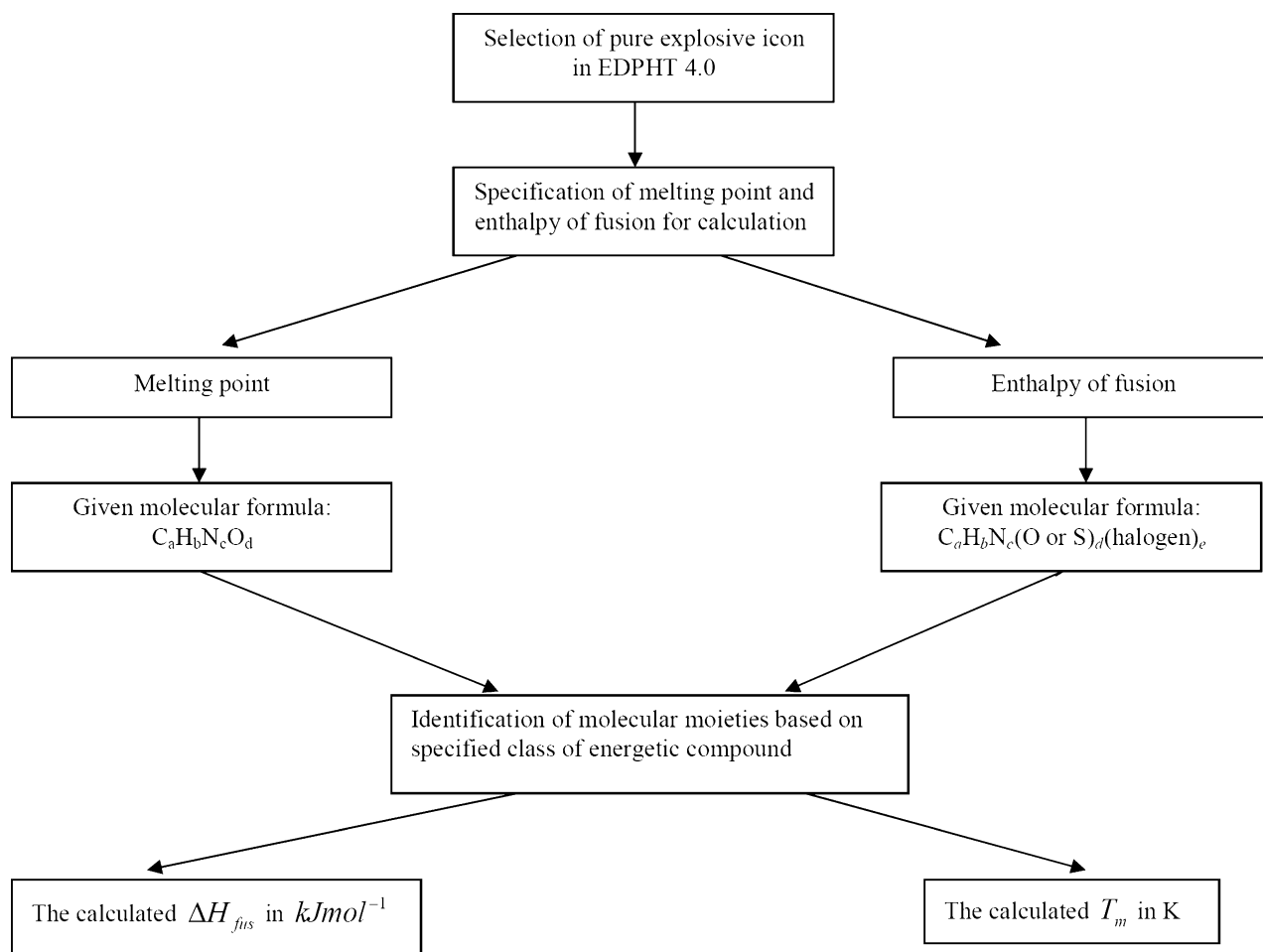


Figure 1. Block diagram of the software EDPHT 4.0.

well as Windows 7.0 and its output can be directly printed. The algorithm of EDPHT 4.0 in prediction of melting point and enthalpy of fusion of pure $C_aH_bN_cO_d$ and $C_aH_bN_c(O \text{ or } S)_d(\text{halogen})_e$ energetic materials, respectively, is shown in Figure 1 as flow chart. The knowledge of the molecular structure of energetic compounds is the only essential parameter, which can be specified as input parameters through empirical formula and specific molecular moieties.

4 Validation of EDPHT 4.0

Some new or well-known explosives of different classes were selected for comparison of the computed values of EDPHT 4.0 with experimental data. The outputs were also compared with well-known methods.

4.1 Predicted Melting Point Values

Table 1 shows the outputs of EDPHT 4.0 for melting points of some new energetic compounds containing complex molecular structures. The calculated data of EDPHT 4.0 are

also compared with two different methods of JR [22] and Jain-Yalkowsky (JY) [25]. The percent of errors for these methods, $[(\text{predicted} - \text{measured}) / \text{measured}] \times 100$, are also given in Table 1. As can be seen in Table 1, the validity of EDPHT 4.0 is in well agreement with both JR [22] and JY [25] methods. Since large deviations generally occur between experimental measurements of melting points by both JR [22] and JY [25] methods, the agreement between outputs of EDPHT 4.0 and measured T_m is also satisfactory. A higher validity of EDPH 4.0 with respect to the other methods may be due to Equation (2) is derived on the basis of experimental data of different classes of energetic compounds.

4.2 Estimation of Enthalpies of Fusion

The calculated enthalpies of fusion of EDPH 4.0 for various well-known and new energetic compounds are given in Table 2. The predicted results of EDPH 4.0 given in Table 2 are also compared with Jain et al. method [23], which is one of the best available empirical methods. As seen in Table 1, the validity of EDPH 4.0 is higher than Jain et al.

Table 1. Comparison of the calculated melting point [K] by EDPHT 4.0 for several new explosives containing complex molecular structures with the measured values.

Name	Formula	Exp.	EDPHT 4.0	% Dev	JR method	% Dev	JY method	% Dev
1,3,5-Trinitro-2,4,6-tripicrylamino benzene	$C_{24}H_9N_{15}O_{24}$	507 [27]	534.4	5.4	2473.0	387.6	1074.3	111.8
1,3,5,5-Tetranitrohexahydropyrimidine (DNNC)	$C_4H_6N_6O_8$	425.65 [28]	402.9	−5.4	812.0	90.8	620.0	45.7
2,4,6-Tris(2-nitroxyethylnitramino)-1,3,5-triazine (Tris-X)	$C_{24}H_9N_{15}O_{24}$	342 [29]	358.3	4.7	343.5	0.4	495.1	44.7
1,3-Bis(1,2,4-triazolo-3-amino)-2,4,6-trinitrobenzene (BTATNB)	$C_{10}H_7N_{11}O_6$	593 [27]	611.7	3.1	1369.0	130.8	898.7	51.5
3,3'-Diamino-2,2',4,4',6,6'-hexanitrodiphenyl (DIPAM)	$C_{12}H_6N_8O_{12}$	577 [27]	518.4	−10.2	1406.0	143.6	836.8	45.0
3,3'-Diamino-2,2',4,4',6,6'-hexanitrodiphenylamine	$C_{12}H_6N_8O_{12}$	508 [29]	535.8	5.5	1458.0	187.2	849.4	67.3
5-Nitro-4,6-bis(5-amino-3-nitro-1H-1,2,4-triazole-1-yl)pyrimidine (DANTNP)	$C_8H_5N_{13}O_6$	609 [27]	635.4	4.3	1415.0	132.3	824.7	35.4
2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20)	$C_6H_6N_{12}O_{12}$	501.15 [28]	493.0	−1.6	1297.8	159.0	757.2	51.1

Table 2. Comparison of the predicted enthalpy of fusion [kJ mol^{−1}] by EDPHT 4.0 for several new explosives containing complex molecular structures with the measured values.

Name	Formula	Exp.	EDPHT 4.0	% Dev	Jain et al.	% Dev
1,5-Diacetyl-3,7-dinitro-1,3,5,7-tetrazocane (DADN)	$C_8H_4N_6O_6$	26.26 [30]	33.30	26.81	43.36	65.12
4,10-Dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane (TEX)	$C_6H_6N_4O_8$	39.81 [30]	30.38	−23.69	27.04	−32.08
		36.18 [30]		−16.03		−25.26
		34.15 [30]		−11.04		−20.82
		34.29 [30]		−11.40		−21.14
2,4,6-Trinitroxylylene	$C_6H_7N_3O_6$	40.87 [32]	28.41	−30.49	18.90	−53.76
Pentaerythritol tetranitrate (PETN)	$C_5H_8N_4O_{12}$	48.05 [33]	48.66	1.27	39.60	−17.59
2,4,6-Triamino-1,3,5-trinitrobenzene (TATB)	$C_6H_6N_6O_6$	56.60 [32]	57.57	1.71	28.72	−49.26
2-Methyl-4-[(3-methyl-2,4,6-trinitrophenyl)thio]-1,3,5-trinitrobenzene	$C_{14}H_8N_6O_{12}S$	57.78 [32]	48.05	−16.84	34.92	−39.56
2,4,7,9-Tetranitro-2,4,7,9-tetraazadecane	$C_6H_{14}N_8O_8$	67.857 [31]	70.18	3.42	43.75	−35.53
		68.448 [31]		2.53		−36.08
		67.975 [31]		3.24		−35.64
		67.975 [31]		3.24		−35.64
2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20)	$C_6H_6N_{12}O_{12}$	42.3 [30]	42.99	1.63	47.90	13.24
		41.12 [30]		4.55		16.49
		44.68 [30]		−3.78		7.21

method [23] because very few energetic compounds were used to develop the method of Jain et al. [23].

As indicated in Table 2, the enthalpies of fusion of new explosives containing complex molecular structures such as 4, 10-dinitro-2,6,8, 12-tetraoxa-4,10-diazatetracyclo (5.5.0.0.5,9 03,11) dodecane (TEX) can be easily calculated. Moreover, the overall agreement of EDPHT 4.0 with reported enthalpy of fusion is quite good for a wide range of different classes of energetic.

4.3 Limitations of EDPHT 4.0

As indicated in Table 1 and Table 2, the new computer code EDPHT 4.0 has relatively good reliability with respect to the best available general methods. However, it has also some restrictions:

(a) EDPHT 4.0 can only predict melting points and enthalpies of fusion of energetic compounds with general formula $C_aH_bN_cO_d$ and $C_aH_bN_c(O \text{ or } S)_d(\text{halogen})_e$, respectively.

(b) Since phase changes of explosives depend on particle size especially nanoscale with respect to macroscale [26], the EDPHT 4.0 can predict melting point and enthalpy of fusion only for macroscale energetic compounds.

5 Conclusions

EDPHT 4.0 can provide an easy to handle computer code for estimation of melting points and enthalpies of fusion of energetic compounds. It requires only elemental composition and some molecular moieties as only input parameters. Several available methods were used to show the higher validity of EDPHT 4.0 for the prediction of melting points and enthalpies of fusion of several new and well-known energetic compounds containing complex molecular structures. Thus, EDPHT 4.0 can be easily applied for new explosive candidates, which require hazardous synthesis, testing, and fielding.

Acknowledgments

The author gratefully acknowledges the research committee of Malek-ashtar University of Technology (MUT) for supporting this work.

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* **2001**, 84, 1.
- [2] J. P. Agrawal, *High Energy Materials: Propellants, Explosives and Pyrotechnics*. Wiley-VCH, Weinheim, **2010**.
- [3] M. H. Keshavarz, Important Aspects of Sensitivity of Energetic Compounds: A Simple Novel Approach to Predict Electric Spark Sensitivity, *Explosive Materials: Classification, Composition and Properties*, (Ed.: T. J. Janssen), Nova Science Publishers, New York, **2011**, pp. 103–123.
- [4] L. E. Fried, W. M. Howard, P. C. Souers. *CHEETAH 2.0 User's Manual*, Lawrence Livermore National Laboratory, Livermore, CA, USA, **1998**.
- [5] H. Muthurajan, R. Sivabalan, M. B. Talawar, S. N. Asthana, Computer Simulation for Prediction of Performance and Thermodynamic Parameters of High Energy Materials, *J. Hazard. Mater. A* **2004**, 112, 17.
- [6] M. H. Keshavarz, H. Motamedoshariati, R. Moghayadnia, H. R. Nazari, J. Azarniamehraban, A New Computer Code to Evaluate Detonation Performance of High Explosives and Their Thermochemical Properties, Part I, *J. Hazard. Mater.* **2009**, 172, 1218.
- [7] M. H. Keshavarz, H. Motamedoshariati, R. Moghayadnia, M. Ghanbarzadeh, J. Azarniamehraban, A New Computer Code for Assessment of Energetic Materials with Crystal Density, Condensed Phase Enthalpy of Formation and Activation Energy of Thermolysis, *Propellants Explos. Pyrotech.* **2013**, 38, 95.
- [8] M. H. Keshavarz, H. Motamedoshariati, R. Moghayadnia, M. Ghanbarzadeh, J. Azarniamehraban, Prediction of Sensitivity of Energetic Compounds with a New Computer Code, *Propellants Explos. Pyrotech.* **2014**, 39, 95.
- [9] L. Gorb, F. C. Hill, Y. Kholod, E. N. Muratov, V. E. Kuz'min, J. Leszczynski, *Progress in Predictions of Environmentally Important Physicochemical Properties of Energetic Materials: Applications of Quantum-Chemical Calculations, Practical Aspects of Computational Chemistry II*, (Eds.: J. Leszczynski, M. K. Shukla), Springer Science, New York, **2012**, pp. 335–359.
- [10] L. N. Ognichenko, V. E. Kuz'min, L. Gorb, E. N. Muratov, A. G. Artemenko, N. A. Kovdienko, P. G. Polishchuk, F. C. Hill, J. Leszczynski, *New Advances in QSPR/QSAR Analysis of Nitrocompounds: Solubility, Lipophilicity, and Toxicity, Practical Aspects of Computational Chemistry II*, (Eds.: J. Leszczynski, M. K. Shukla), Springer Science, New York, **2012**, pp. 279–334.
- [11] E. Poling, J. M. Prausnitz, J. P. O'Connell, *The Properties of Gases and Liquids*, McGraw-Hill, London, **2001**.
- [12] M. H. Keshavarz, Approximate Prediction of Melting Point of Nitramines, Nitrate Esters, Nitrate Salts and Nitroaliphatics Energetic Compounds, *J. Hazard. Mater. A* **2006**, 138, 448.
- [13] M. H. Keshavarz, Predicting Heats of Fusion of Nitramines, *Ind. J. Eng. Mater.* **2007**, 14, 386.
- [14] M. H. Keshavarz, H. R. Pouretedal New Approach for Predicting Melting Point of Carbocyclic Nitroaromatic Compounds, *J. Hazard. Mater. A* **2007**, 148, 592.
- [15] M. H. Keshavarz, A Simple Correlation for Predicting Heats of Fusion of Nitroaromatic Carbocyclic Energetic Compounds, *J. Hazard. Mater.* **2008**, 150, 387.
- [16] M. H. Keshavarz, New Method for Predicting Melting Points of Polynitro Arene and Polynitro Heteroarene Compounds, *J. Hazard. Mater.* **2009**, 171, 786.
- [17] R. Fareghi Alamdari, M. H. Keshavarz, A Simple Method to Predict Melting Points of Non-Aromatic Energetic Compounds, *Fluid Phase Equilib.* **2010**, 292, 1.
- [18] A. Semnani, M. H. Keshavarz, Using Molecular Structure for Reliable Predicting Enthalpy of Melting of Nitroaromatic Energetic Compounds, *J. Hazard. Mater.* **2010**, 178, 264.
- [19] M. H. Keshavarz, Prediction of Enthalpy of Fusion of Non-aromatic Energetic Compounds Containing Nitramine, Nitrate and Nitro Functional Groups, *Propellants Explos. Pyrotech.* **2011**, 36, 42.
- [20] M. H. Keshavarz, F. Gharagheizi, H. R. Pouretedal, Improved Reliable Approach to Predict Melting Points of Energetic Compounds, *Fluid Phase Equilib.* **2011**, 308, 114.
- [21] Y. Mosaei Oskoei, M. H. Keshavarz, Improved Method for Reliable Predicting Enthalpy of Fusion of Energetic Compounds, *Fluid Phase Equilib.* **2012**, 326, 1.
- [22] K. G. Joback, R. C. Reid, Estimation of Pure-Component Properties from Group-Contributions, *Chem. Eng. Commun.* **1987**, 57, 233.
- [23] A. Jain, G. Yang, S. H. Yalkowsky, Estimation of Melting Points of Organic Compounds, *Ind. Eng. Chem. Res.* **2004**, 43, 7618.
- [24] P. Simamora, S. H. Yalkowsky, Group Contribution Methods for Predicting the Melting Points and Boiling Points of Aromatic Compounds, *Ind. Eng. Chem. Res.* **1994**, 33, 1405.
- [25] A. Jain, S. H. Yalkowsky, Estimation of Melting Points of Organic Compounds-II, *J. Pharm. Sci.* **2006**, 95, 2562.
- [26] N. Zohari, M. H. Keshavarz, S. A. Seyedsadjadi, The Advantages and Shortcomings of Using Nano-Sized Energetic Materials, *Cent. Eur. J. Energ. Mater.* **2013**, 10, 135.
- [27] J. P. Agrawal, Recent Trends in High Energy Materials, *Prog. Energy Combust. Sci.* **1998**, 24, 1.
- [28] P. F. Pagoria, J. S. Lee, A. R. Mitchell, R. D. Schmidt, A Review of Energetic Materials Synthesis, *Thermochim. Acta* **2002**, 384, 187.
- [29] J. P. Agrawal, R. D. Hodgson, *Organic Chemistry of Explosives*, John Wiley & Sons, New York, **2007**.
- [30] S. Zeman, Z. Jalový, Heats of Fusion of Polynitro Derivatives of Polyazaisowurtzitane, *Thermochim. Acta* **2000**, 345, 31.
- [31] S. Zeman, Some Predictions in the Field of the Physical Thermal Stability of Nitramines, *Thermochim. Acta* **1997**, 302, 11.
- [32] 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. Pyrotech.* **2003**, 28, 301.
- [33] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th Ed. Wiley-VCH, Weinheim, **2007**.

Received: February 9, 2014

Revised: April 24, 2014

Published online: June 2, 2014