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# Calculated Lattice Energies of Energetic Materials in a Prediction of their Heats of Fusion and Sublimation

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Abstract: The paper specifies an unambiguous basic relationship between the published results of *ab initio* calculations of lattice energies,  $E_{\rm L}$ , and heats of sublimation,  $\Delta H_{\rm s}$ , of individual energetic materials. In this relationship, the  $\Delta H_{\rm s}$  value has been replaced by heats of fusion,  $\Delta H_{\rm m,tr}$ . Thereby its unambiguity has been lost, and the similarity of details of molecular structure begins to be of decisive importance. The resulting partial relationships, together with the basic relationship, have been used for prediction of  $\Delta H_{\rm s}$ , and  $\Delta H_{\rm m,tr}$  values of technically attractive polynitro compounds.

Key words: polynitro compound; heat of fusion; heat of sublimation; lattice energy; DSC CLC number: 0642.3; TQ560.7 Document code: A

# **1** Introduction

The studies of the relationship between molecular structure of energetic materials and their sensitivity to impact, shock, electric spark and heat form an important starting point for study of chemical micromechanism governing detonation initiation of these materials<sup>[1~8]</sup>. From the results of studies it follows that the intensity of intermolecular interactions in the corresponding crystal represents one of the factors influencing the transfer of initiation energy into the reaction centre of the molecule<sup>[1-7]</sup>. This fact is documented by the findings obtained from studies of impact<sup>[1-3,7]</sup> or electric spark initiations<sup>[4-7]</sup> of polynitro compounds. According to Ref. [8], the thermal decomposition or the initiation of detonation of nitramines should be accompanied by primary homolysis of those nitramino groups in their molecules that contribute in decisive way to intermolecular potential in the respective crystals. The effects of intermolecular influences or state of aggregation on thermal decomposition of energetic materials are well known (e. g., see Refs.  $\lceil 9 \sim 11 \rceil$  and the citations given therein).

From among the measurable quantities the heat of sublimation is the best parameter as far as the characteristic of the intensity of intermolecular interactions within a crystal is concerned. However, the respective values of many energetic materials have not been published yet. Nevertheless, in some specific cases it is possible to replace the heat of sublimation by the heat of fusion<sup>[1~3,8]</sup>, determined with the help of DSC. Recently, it has also been possible to get an idea of the said interactions from *ab initio* calculations of the lattice energies, as shown by Thompson et al. for about 80 individual energetic materials<sup>[12,13]</sup>. The above-mentioned approaches and findings<sup>[1~3,8,12,13]</sup>, complemented by several new results from DSC, have been used in the present paper to predict the heats of fusion and sublimation of some both technically attractive and theoretically interesting polynitro compounds.

### 2 Experimental

The heats of fusion,  $\Delta H_{m,tr}$ , (according to monograph<sup>[14]</sup> defined as the sum of heat of melting and heats of all polymorph transitions) were determined by means of a Perkin-Elmer differential scanning calorimeter Pyris DSC 7. The apparatus was calibrated for indium and lead. During the measurement, nitrogen was introduced into the furnace of the DSC and the heating rate of 20 °C · min<sup>-1</sup> was used. Weighed amounts (0. 897 ~ 2.064 mg) of crystalline polynitro compounds were placed in aluminum pans (Perkin-Elmer, Part No. BO14-3016) fitted with covers (Perkin-Elmer, Part No. BO143040). The DSC records were analyzed by means of the Pyris series thermal analysis software (Perkin-Elmer, Part No. N557-0600), which is licensed by Perkin-Elmer. The

results of measurements are summarised in Table 1 along with the published data of heats of fusion<sup>[3,8,11,15-20]</sup>, heats of sublimation<sup>[18,21-25]</sup> and lattice energies<sup>[12,13]</sup>.

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Table 1	Survey of the substances studied	their beats of fusion and	auhlimation and	latting anonging
I able I	Survey of the substances studied.	their neats of fusion and	i submination and	lattice energies
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Substance		DSC onset		Heat of		Heat of		Lattice energy $E_{\rm L}$		
	•		/	′К	fusion	n	sublim	ation	/kJ • mol	
Data No.	Chemical name	Code designation	polymor transitio	ph melting	$\int \Delta H_{m,tr}$ /kJ · mol <sup>-1</sup>	Ref.	$\Delta H_s$ /kJ • mol	-1 Ref.	predicted value [12,13] <sup>a</sup>	adapted value
1. 1	1,3,5-Trinitrobenzene	TNB	.61	396.2	15.69	11	107.3	21	-132.55, -123.69 -118.11, -114.48	- 122.58 <sup>b</sup>
1. 2	· · · · · · · · · · · · · · · · · · ·	NN	4		16.74	15				- 127. 30 <sup>f</sup>
2. 1	1-Methyl-2,4,6-trinitrobenzene	TNT			21.86	16	118.4	22	- 151.98, - 141.49 - 135.57, - 130.97	– 136. 11 <sup>b</sup>
2. 2				353.2	19.58	с				- 137. 43 <sup>f</sup>
2. 3							113.2	21		- 129.77 <sup>b</sup>
3. 1	1,3-Dimethyl-2,4,6-trinitrobenzene	TNX		454.4	40.87	с	129.8	21		- 150.00 <sup>b</sup>
4.	1,3,5-Trimethyl-2,4,6-trinitrobenzene	TNMs		512.4	30.72	с	103.6	21		- 118.07 <sup>b</sup>
5. 1	1-Hydroxi-2,4,6-trinitrobenzene	PA		394.1	17.41	с			- 152.55, - 141.58 - 135.30, - 129.16	- 129.69 <sup>f</sup>
5. 2							105.1	21		- 119. 90 <sup>b</sup>
6. 1	1,3-Dihydroxi-2,4,6-trinitrobenzene	TNR		450.4	28.80	с	120.8	21		- 139.04 <sup>b</sup>
7. 1	1-Methyl-3-hydroxi-2, 4, 6-trinitro- benzene	TNCr	379.1	386.0	26.74	с	111.2	21		- 143.70 <sup>b</sup>
8. 1	1-Amino-2,4,6-trinitrobenzene	PAM		465.4	28.15	с	125.3	21		- 144. 52 <sup>b</sup>
9. 1	1-(N,N-Dimethylamino)-2,4,6-trinitro- benzene	DMPAM		439.32	34.71	с	116.6	b	- 148.23, - 140.90 - 138.97, - 135.27	- 133. 94 <sup>g</sup>
10. 1	1,3-Diamino-2,4,6-trinitrobenzene	DATB	500.2	560.8	35.25	с	140.0	23		- 162. 43 <sup>b</sup>
11. 1	1,3,5-Triamino-2,4,6-trinitrobenzene	ТАТВ	als	594 <sup>d</sup>	56.60	e	168.2	23		- 196.80 <sup>b</sup>
12. 1	2,4,6-Trinitrobenzoic acid	TNBA		502.3	31.60	с	154.7	b		- 180. 33 <sup>f</sup>
13. 1	2,2',4,4',6,6'-Hexanitrobiphenyl	HNB		517.1	37.44	11	171.8	b		-201.17 <sup>f</sup>
14. 1	3,3'-Dimethyl-2,2',4,4',6,6'-hexanitro- biphenyl	BITNT		514.7	33.69	с	160.8	b		- 187.79 <sup>f</sup>
15. 1	2,2',4,4',6,6'-Hexanitrodiphenylsulfide	DIPS	453.9	506.1	38.00	с	173.4	b		- 203. 17 <sup>f</sup>
16. 1	2,2',4,4',6,6'-Hexanitrostilbene	HNS		585 dec.	40.21	f	179.9	23	-257.38, -238.13 -225.41, -216.36	-211.06 <sup>b</sup>
17. 1	2,2',4,4',6,6'-Hexanitrodiphenylamine	DPA		524.3	37.38	с	171.6	b		- 200. 96 <sup>f</sup>
18. 1	1-(2, 4, 6-trinitrophenyl)-5, 7-dinitro- benzotriazole	BTX		529	40.10	26	179.7	b	-226.63, -212.98 -206.47, -202.42	-210.88 <sup>f</sup>
19. 1	1,8-Dinitronaphthalene	1,8-DNN	397.6	444.5	35.23	с			-139.38, -131.59 -126.66, -123.25	
20. 1	Trinitromethane	TNM					54.8	20	-60.10, -53.50 -50.83, -49.38	- 58.6 <sup>b</sup>

		Та	able 1	( Continue	d)				CU	
Substance			DSC onset		Heat of		Heat of		Lattice energy $E_{\rm L}$	
	Substance			/ K	fusion		sublimation C		/kJ · mol	1
Data No.	Chemical name	Code designation	polymo transiti	on melting	$\Delta H_{\rm m,tr}$ /kJ · mo	$l^{-1}$ Ref.	$\Delta H_s$ /kJ · mol	Ref.	predicted value $[12,13]^{a}$	adapted value
21. 1	1-Nitro-1-azaethylene	<b>DIGEN</b> <sup>1</sup>		368.5 <sup>k</sup>	23.45	3	85.7	b	T	-96.22 <sup>i</sup>
22. 1	2-Nitro-2-azapropane	DMNA		328.3	17.26	17	69.9	22	-70.26, -71.20 -70.21, -76.25	$-77.00^{\mathrm{b}}$
23. 1	1,3,5-Trinitro-1,3,5-triazacyclohexane	RDX	~	476.4	33.01	17	130.2	18	- 130.09, - 133.68 - 136.05, - 148.18	- 131.03 <sup>b</sup>
24. 1	1,3-Dinitro-1,3-diazacycloheptane	1,3-DNHp	369	376	27.40	19	107.3	b	- 120.00, - 122.66 - 122.20, - 131.95	- 122.56 <sup>h</sup>
25. 1	1,3,5-Trinitro-1,3,5-triazacycloheptane	номо	425.2	433.6	27.74	3	108.6	b		- 124. 22 <sup>h</sup>
26. 1	trans-1, 4, 5, 8-Tetranitro-1, 4, 5, 8-tet- raazadecaline	TNAD		decomp. at 470	46.40	17	154.2	b	- 169.22, - 172.11 - 177.36, - 190.98	- 179. 80 <sup>i</sup>
27. 1	1,4-Dinitro-1,4-diazacyclobutane	<b>TETROGEN</b> <sup>1</sup>		433.8 <sup>k</sup>	26.32	23	94.2	b		- 106. 67 <sup>i</sup>
28. 1	1,3,3-Trinitroazetidine	TNAZ		372.1	30.31	20	63.2	25	- 113.01, - 116.40 - 118.81, - 129.07	- 121.20 <sup>i</sup>
28. 2							106.2	b		
29. 1	1,5-Endomethylene-3,7-dinitro-1,3,5,7- tetraazacyclooctane	DPT		decomp. at 433.3	28.16	3	132.4	b	- 140.60, - 142.78 - 142.60, - 154.30	- 153. 14 <sup>j</sup>
30. 1	1, 5-Diacetyl-3, 7-dinitro-1, 3, 5, 7-tet- raazacyclooctane	DADN		decomp. at 497.1	25.76	3	142.4	b		- 165. 42 <sup>j</sup>
31. 1	1,3,5,7-Tetranitro-1,3,5,7-tetraaza-cy- clooctane	β-HMX	457.7	decomp. at 547.9	32.10	17	175.3	16	- 180. 23, - 185. 02 - 187. 01, - 204. 45	- 183.25 <sup>b</sup>
32. 1	1,3,5,7,9-Pentanitro-1,3,5,7,9-pentaa- za-cyclodecane	DECAGEN <sup>1</sup>		600.3 <sup>k</sup> decomp.	34.93	1,3	120.0	b		- 138. 03 <sup>i</sup>
33. 1	2,4,6,8,10,12-Hexanitro-2,4,6,8,10, 12-hexaazaisowurtzitane	$\varepsilon$ -HNIW	437.3	decomp. at 480.1	42.70	8	168.7	b	- 186.77, - 192.82 - 196.52, - 210.88	- 197.40 <sup>h</sup>
34. 1	4,10-Dinitro-2,6,8,12-tetraoxa-2,4,6,8, 10,12-hexaazaisowurtzitane	TEX		598 dec. 600	36.10	8	123.4	b		- 142. 29 <sup>i</sup>
35. 1	1-Methylnitramino-2, 4, 6-trinitro-ben- zene	TETRYL		400.5	25.85	19	133.8	21	- 149.53, - 153.81 - 158.30, - 170.57	- 171.24 <sup>b</sup>
36. 1	Pentaerythritol tetranitrate	PETN	1G	old.			151.9	24	- 178.65, - 166.87 - 161.77, - 156.84	– 176. 94 <sup>b</sup>
36. 2		ri	912				150.4	21		- 175. 10 <sup>b</sup>

Notes: a) The values predicted<sup>[12,13]</sup> by means of the *ab initio* models: MP2/6 - 31G<sup>\*\*</sup>, B3LYP/6 - 31G<sup>\*\*</sup>, 0.9HF/6 - 31G<sup>\*\*</sup> and HF/6 - 31G<sup>\*\*</sup>;

b) Calculated by means of relationship from Fig. 1;

c) The value resulted from DSC measurement in this paper;

d) The value taken from Ref.  $\left[\,27\,\right]$  ;

e) Calculated by means of relationship B from Fig. 3;

f) Calculated by means of relationship from Fig. 2;

g) Calculated by means of relationship A from Fig. 3;

h) Calculated by means of relationship B from Fig. 4;

(Fi) Calculated by means of relationship A from Fig. 4;

j) Calculated by means of relationship C from Fig. 4;

k) Predicted value, taken from Ref.  $\left[\,17\,\right]$  ;

1) The nitramine has not been synthesized yet.

# **3** Results and Discussion

A comparison of the published values of heats of sublimation,  $\Delta H_s$ , and the calculated values of lattice energies,  $E_{\rm L}$ , resulted in the expected linear relationship  $E_{\rm L} = a\Delta H_s + b$  (1) which is demonstrated in Fig. 1. With the use of the published  $\Delta H_s$  values and Eq. (1), the results of *ab initio* calculations of the individual substances were "averaged" (see adapted  $E_{\rm L}$  values in Table 1), and the  $E_{\rm L}$  values so far not calculated were assessed as helpful mathematical values. The data of TNAZ do not correlate in the sense of Eq. (1), which is due to the non-realistically low value of

its published  $\Delta H_s$  (see Table 1). The value of  $\Delta H_s$  is 106.2 kJ  $\cdot$  mol<sup>-1</sup>, predicted here for this substance, falls within the expected limits<sup>[28]</sup>.

In the context of partial findings from Refs.  $[1 \sim 3, 8]$ , we have made an attempt at substitution of  $\Delta H_s$  value in Eq. (1) by the heat of fusion,  $\Delta H_{m,tr}$ , which resulted in the general equation

$$E_{\rm L} = a_1 \Delta H_{\rm m,tr} + b_1 \tag{2}$$

As the Figs. 2,3 and 4 show, this equation is valid within narrow molecular-structural series. On the basis of Eq. (2), we predicted the  $E_{\rm L}$  helpful values and then-with application of Eq. (1) - also the  $\Delta H_{\rm s}$  values of some substances from Table 1.



Fig. 2 Graphic representation of Eq. (2) for a part of 1,3,5 - trinitrobenzene derivatives



Fig. 3 Graphic representation of Eq. (2), constructed on the basis of "averaged" results of *ab initio* calculations and assessed  $E_{\rm L}$  values for polynitro arenes; in the case of DMPAM the highest  $E_{\rm L}$  values from *ab initio* calculation were taken (see Table 1)



The above-mentioned validity of Eq. (2) for a part of 1,3,5-trinitrobenzene derivatives is illustrated by Fig. 2: here data 9.1 do not correlate with those of the said derivatives due to a steric influence of the N,N-dimethylamino grouping upon conformation of the corresponding DMPAM molecule (more about conformation of the N,Ndisubstituted polynitroanilines see in Refs. [29,30]). Data 19.1 cannot correlate with line in Fig. 2 because they correspond to a naphthalene derivative, i. e. 1,8-DNN.

Lines in Fig. 3 we have constructed by means of "averaged" results of *ab initio* calculations (i. e. adapted values from Table 1) and assessed  $E_{\rm L}$  helpful values. According to the Figure the polynitro arenes studied are logically divided in several subsets on the basis of similarity details of their molecular structure. Subset A in this

Figure represents sterically fairly hindered molecules TNX, TNMs and DMPAM whose data do not correlated with data of TNB. On the basis of relationship for subset B a realistic assessment of the  $\Delta H_{m,tr}$  value for TATB we have made (see data 11.1). Subset C contains dipicryl derivatives. As the monocarboxylic acids in their crystalline state forms dimers (through carboxyl grouping), the data 12.1 of 2,4,6-trinitrobenzoic acid perfectly correlate with relationship for subset C in Fig. 3.

Similar approach, as that used in the case of Fig. 1, we have also adopted in Fig. 4 to "average" the results of ab initio calculations of individual nitramines and, by means of Eq. (2), to assess the  $E_{\rm L}$  values so far not calculated (see Table 1). On the basis of similarity of molecular structure the group of the nitramines studied can be divided into three logical subsets in the sense of Eq. (2). Taking some knowledge from the study of heat of fusion in nitramines series<sup>[8]</sup> we have used a relationship for subset A in Fig. 4 for an assessment of the  $E_{\perp}$  helpful values in the data 21.1,27.1,32.1 and 34.1. Relatively low predicted  $E_{\rm L}$  and  $\Delta H_{\rm m,tr}$  values in the data 32.1 (i. e. for DECAGEN), regarding to those for HMX and RDX, can connect with high stressing in DECAGEN molecule (about this stressing see in Ref. [31]): it was shown<sup>[31]</sup> that the highly stressed molecules of cyclic nitramines form crystals of lower densities than their less stressed analogues ( both the  $E_{\rm L}$  and  $\Delta H_{\rm m,tr}$  values have a relation to theoretical maximum densities of RDX, HMX and DECAGEN crystals). As the HNIW molecule contains triazacycloheptane skeleton, we have used subset B of nitramines for a prediction of the  $E_{\perp}$  helpful value of 1, 3,5-trinitro-1,3,5-triazacycloheptane (data 25.1). Subset C in Fig. 4 corresponds to 1, 3, 5, 7-tetraazacyclooctane derivatives and, therefore, we have taken corresponding relationship for an assessment of the  $E_{\rm L}$  helpful values of DADN.

# 4 Conclusions

In accordance with what was expected there exists an unambiguous linear dependence between the results of *ab initio* calculations of lattice energies according to Thompson et al. <sup>[12,13]</sup> and the heats of sublimation,  $\Delta H_s$ , of the individual energetic materials. If the  $\Delta H_s$  values in this

basic dependence are replaced by the heats of fusion,  $\Delta H_{m,tr}$ , its unequivocality is lost, and the similarity of detailed molecular structure becomes decisive (the studied set of energetic materials being divided into narrow subseries of compounds with the look-alike molecular structure). The corresponding partial relationships together with the basic dependence offer relatively wide possibilities of prediction of both the heats of sublimation or fusion. From the point of view of these characteristics the most stable polynitro compounds from studied energetic materials in this paper may be arranged in the order of decreasing stability: HNS > BTX >  $\beta$ -HMX.

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