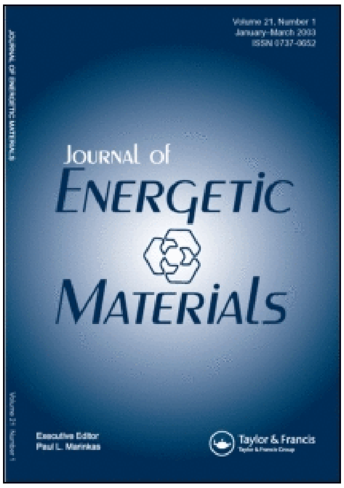

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A New View of Relationships of the N–N Bond Dissociation Energies of Cyclic Nitramines. Part II. Relationships with Impact Sensitivity

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The values of bond dissociation energies, BDE, of the weakest N–N bonds and total energies, E_{total}, of molecules have been calculated for 14 cyclic nitramines by means of the UB3LYP/6-31G and UB3LYP/6-31+G* // PM3 methods. The relationships found between the BDE values and logarithms of impact sensitivity of these nitramines, expressed as drop energy, E_{dr}, are not unambiguous. Replacement of these BDE values by the BDE/E_{total} ratio has not resulted in any simplification of the said relationships, but their quality improved, particularly with application of the UB3LYP/6-31+G* // PM3 (UHF) method. The reason of ambiguity of the relationships found mainly lies in real conformation of the respective molecules and intermolecular force effects in*

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real molecular crystals, which are included in neither of the two calculation methods.

Keywords: bond dissociation energy, cyclic nitramines, impact sensitivity

Introduction

Studies of the sensitivity of energetic materials are inseparably connected with the understanding of the primary chemical processes of their initiation. Over the last 10 years the study of problems of this sensitivity (i.e., initiation reactivity) has accelerated thanks to theoretical methods based on quantum chemistry. Impact and shock sensitivities have been in the center of interest [1]. The dissociation energy of the weakest bond in the molecule of energetic material is thought to play an important role in the initiation events. However, some authors accept the idea that the correlation between bond strength and impact sensitivity is not generally limited within certain classes of molecules [2,3]. Fried et al. [3] state that the energy content of the material must also play a role in determining the impact sensitivity. Hence, for a characteristic of the impact sensitivity (impact reactivity) the authors introduce the ratio of bond dissociation energy (*BDE*) and energy content, E_d, calculated by means of CHEETAH [3]. The authors have presented an unambiguous semi-logarithmic relationship between this ratio BDE/E_d and impact sensitivity, expressed as log $h_{50\%}$ [3] ($h_{50\%}$ stands for drop height), for 14 various polynitro compounds containing C–NO_2, N–NO_2, and O–NO_2 bonds in their molecules; however, this published relationship lacks basic statistical characteristics. Song et al. [4] modified the previous relationship replacing the E_d values by the total energy of molecule, E_{total} (calculated by means of B3LYP 6-31G*) and applied it successfully to 5 derivatives of geminal polynitro paraffin derivatives (i.e., to compounds of a single type having about the same configurations of the reaction center of molecule).

In our experience, the problem is not as clear as it appears in the above-given statements (e.g., Fried et al. [3] and Song et al. [4]). Therefore, our study is dedicated to the relationship between impact sensitivity of 14 cyclic nitramines (i.e., compounds seemingly of a single sort) and the *BDE* values of the weakest bonds in their molecules and the values of their BDE/E_{total} ratios.

Substances and Data

Table 1 presents a set of the cyclic nitramines and their impact sensitivity data. Purity of the nitramines tested in this study was checked by means of HPLC. For the sensitivity determination, the standard impact tester with exchangeable anvil [5,6] was adopted, the amount of tested substance being 40 mm^3 [5], detection on the basis of sound (the Bruceton method [6,7,9]); 1- and 2-kg weight drop hammers were used [5,6]. Using the up-and-down method, the obtained sensitivity was expressed as the drop energy, E_{dr} [5,6]; a part of the E_{dr} values was taken from the literature [7–12]. All the E_{dr} values are presented in Table 1. This table also presents the heats of fusion, $\Delta H_{m,tr}$, taken from Atalar and Zeman [13]; for a given substance these values represent a sum of heats of all polymorphic transitions and the heat of melting [14]. Table 1 also presents nitramines tetrogen and decagon, which have not been synthesized yet; their properties were predicted earlier (see Zeman and Krupka [7] and Zeman [15,16] and references therein).

Table 2 presents calculated total energies, E_{total}, of the investigated nitramines and their fragments as a result of N–NO_2 bond rupture and the value of the bond dissociation energies (*BDE*s) of the weakest N–N bonds in the molecules of the nitramines studied. The calculations of *BDE*s were performed by means of the UB3LYP/6-31G* and UB3LYP/6-31+G* // PM3 (UHF) methods [17,18]; the values obtained by these two methods for isolated molecules are denoted by the codes BDE^a and BDE^b, respectively. All the calculations were performed by using Spartan 06 package program. Table 2 also includes the dimensionless ratios DBE/E_{total}, denoted as *Ratio*. As already stated, the application of the *Ratio* in this article was taken from Song et al. [4].

Table 1

A survey of the studied cyclic nitramines and their impact sensitivity expressed as the drop energy, E_{dr}, and their heats of fusion, $\Delta H_{m,tr}$ (see Atalar and Zeman [13] and references therein)

Data no.	Chemical name of nitramine	Code designation	Impact sensitivity		Heat of fusion [13] $\Delta H_{m,tr}$ (kJ mol^{-1})
			E_{dr} (J)	Ref.	
1	1,3-Dinitro-1,3-diazetidine	Tetrogen	9.97	7	26.32
2	1,3,3-Trinitroazetidine	TNAZ	6.90	9	30.31
3	1,3-Dinitroimidazolidine	CPX	17.96	[a]	22.57
4	1,4-Dinitropiperazine	DNDC	11.67	[a]	33.82
5	1,3,5-Trinitro-1,3,5-triazinane	RDX	5.58	8	33.01
6	1,3,5-Trinitro-1,3,5-triazepane	HOMO	4.55	[a]	27.73
7.1	*β*-1,3,5,7-Tetranitro-1,3,5,7-tetrazocane	*β*-HMX	6.37	8	32.10
7.2	*α*-1,3,5,7-Tetranitro-1,3,5,7-tetrazocane	*α*-HMX	1.93	[a]	32.10
8	*cis*-1,3,4,6-Tetranitrooctahydroimidazo [4,5-d]-imidazole	BCHMX, bicyclo-HMX	2.98	[a]	31.89

(*Continued*)

Table 1
Continued

Data no.	Chemical name of nitramine	Code designation	Impact sensitivity E_{dr} (J)	Impact sensitivity Ref.	Heat of fusion [13] $\Delta H_{m,tr}$ (kJ mol^{-1})
9	*trans*-1,4,5,8-Tetranitrodecahydro-pyrazino[2,3-*b*]-pyrazine	TNAD	8.58	10	46.40
10	1,3,5,7,9-Pentanitro-1,3,5,7,9-pentazecane	Decagen	4.90	7	34.93
11.1	ε-2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane	ε-HNIW	11.90	11	43.03
11.2	α-2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane	α-HNIW	10.20	11	43.03
12	4,8,10,12-Tetranitro-2,6-dioxa-4,8,10,12-tetraaza-isowurtzitane	Aurora-5, TNIW-5	12.54	[b]	41.73
13	4,6,10,12-Tetranitro-2,8-dioxa-4,6,10,12-tetraaza-isowurtzitane	Aurora-6, TNIW-6	12.16	[b]	41.67
14	4,10-Dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane	TEX	23.00	12	36.10

[a] The value measured in this article.
[b] The value predicted in this article (see Table 3).

Table 2

A survey of the results of calculations by means of the UB3LYP/6-31G* and UB3LYP/6-31 + G* // PM3 (UHF) methods; total energies, E_{total}, of molecules of the considered nitramines and of fragments R and bond dissociation energy values, *BDE*s, of the weakest N–N bonds

	UB3LYP/6-31G* method			UB3LYP/6-31 + G*// PM3 method		
Nitramine	Total molecular energy E_{total} (a.u.)	BDE^a (kJ mol^{-1})	$Ratio^a$ (10^{-5})	Total molecular energy E_{total} (a.u.)	BDE^b (kJ mol^{-1})	$Ratio^b$ (10^{-5})
1. Tetrogen	−598.145870	145.794	9.284	−598.250756	147.742	9.406
1 R	−393.026959			−393.112507		
2. CPX	−637.462307	142.643	8.544	−637.592981	134.252	8.020
2 R	−432.344596			−432.459870		
3. TNAZ	−786.600738			−786.727902		
3 R (N–N)	−581.476374	160.111	7.753	−581.585436	158.814	7.689
3 R (C-N)	−581.474480	165.084	7.994	−581.580755	171.104	8.284
4. DNDC	−676.756808	171.046	9.627	−676.921350	179.119	10.078
4 R	−471.628279			−471.771150		
5. RDX	−897.265511	153.552	6.537	−897.418043	144.471	6.132
5 R	−692.143645			−692.281040		
6. HOMO	−936.551276	152.158	6.188	−936.730074	145.353	5.910
6 R	−731.429941			−731.592735		

(*Continued*)

Table 2
Continued

	UB3LYP/6-31G* method			UB3LYP/6-31 + G*// PM3 method		
Nitramine	Total molecular energy E_{total} (a.u.)	BDE^{a} (kJ mol^{-1})	$Ratio^{a}$ (10^{-5})	Total molecular energy E_{total} (a.u.)	BDE^{b} (kJ mol^{-1})	$Ratio^{b}$ (10^{-5})
7. HMX	−1196.354948	153.715	4.894	−1196.546670	135.599	4.316
7 R	−991.233020			−991.413046		
8. BCHMX	−1195.165324	140.291	4.471	−1195.339070	131.892	4.203
8 R	−990.048509			−990.206858		
9. TNAD	−1273.722908	137.001	4.097	−1273.923260	98.359	2.941
9 R	−1068.607346			−1068.803820		
10. Decagen	−1495.444899	148.648	3.786	−1495.663440	107.496	2.738
10 R	−1290.324901			−1290.540520		
11. HNIW	−1790.961447	148.895	3.167	−1791.187680	139.947	2.976
11 R	−1585.841355			−1586.052400		
12. Aurora-5	−1421.779884	146.101	3.914	−1421.982960	165.414	4.431
12 R	−1216.660856			−1216.837980		
13. Aurora-6	−1421.778269	146.805	3.933	−1421.978700	152.419	4.083
13 R	−1216.658973			−1216.838670		
14. TEX	−1052.595046	173.133	6.265	−1052.775060	166.801	6.035
14 R	−847.465722			−847.629552		
NO_2	−205.063381			−205.081977		

$Ratio = BDE/E_{\text{total}}$ and $BDE = [E(\text{RNO}_2) + E(\text{NO}_2)] - E(\text{R–NO}_2)$.

Results and Discussion

It is well known that intra- and intermolecular interactions in crystals affect the conformation of molecules as compared with the conformation of the same isolated molecules (conditions of the *BDE*s calculation) or in solution or melt (some N–N bonds in crystals of nitramines can be compressed [19]). In the case of nitramino grouping acting as a carrier of orientation interaction in nitramine crystals, one of the N–N bonds is usually the longest one [19–21]. The influence of these intermolecular interactions has been studied most reliably on the example of thermal decomposition of polynitro compounds, where it is known as a stabilizing effect of crystal lattice [22,23] or also as a retardation effect of crystal lattice (REL) [24]; the said effect acts against formation of the activated complex of the reaction and, as it were, increases the strength of the weakest (the most reactive) bond in the molecule. From the results of studies of this type it follows that both the intensity of intermolecular interactions [1,15,25] and dislocations [26] in the corresponding crystal represent the factors influencing the transfer of initiation energy into the reaction center of the molecule.

The said facts can represent one reason from among the main reasons that lead to the complicated semi-logarithmic relationship between the *BDE* values and impact sensitivity in Figs. 1 and 2. In these diagrams, the straight lines with positive slope represent the expected logical relationship between *BDE* and impact sensitivity. The mutual difference between the individual solid lines in each diagram can be due to the differences in intensity of intermolecular interactions in crystal, as considered on the basis of heats of fusion, $\Delta H_{m,tr}$ (i.e., on the basis of the work needed for formation of defects in crystal lattice). The substances involved in straight lines A and E (except for tetrogen in Fig. 1) exhibit the $\Delta H_{m,tr}$ values in the range of 36.1–46.4 kJ mol^{-1}; on the other hand, the $\Delta H_{m,tr}$ values for substances involved in straight lines B and F lie in the range of 27.7–33.8 kJ mol^{-1}. This begs the question whether the data of tetrogen in Fig. 1 belong only to straight line C (compare with straight line G in Fig. 2). Straight lines C and G strictly

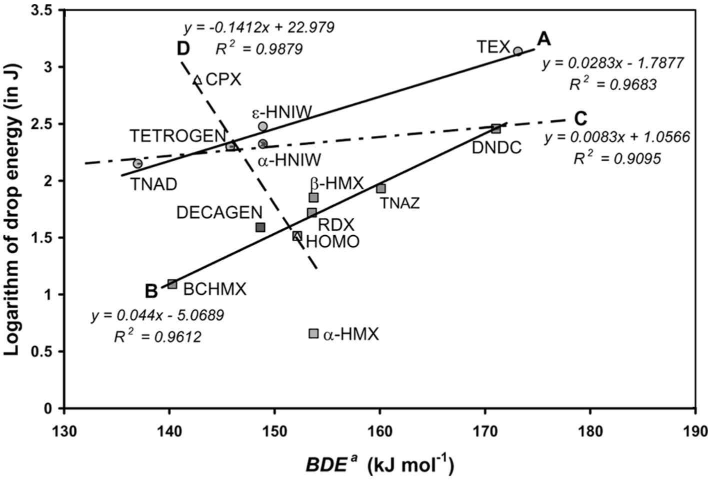


Figure 1. Semi-logarithmic relationship between BDE^a, obtained by UB3LYP/6-31G* method, and impact sensitivity (expressed as drop energy) of the studied nitramines.

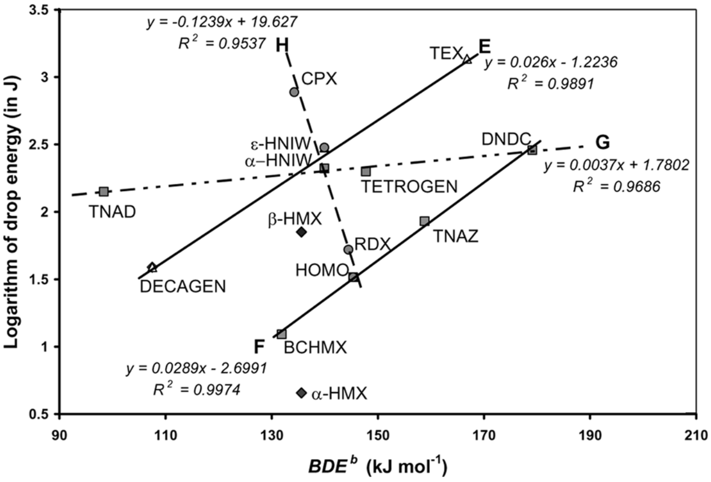


Figure 2. Semi-logarithmic relationship between BDE^b, obtained by UB3LYP/6-31+G* // PM3 method, and impact sensitivity (expressed as drop energy) of the studied nitramines.

result from the presence of the piperazine skeleton in the molecules of TNAD and HNIW; this skeleton can notionally be derived by symmetrical introduction of two methylene groups into the molecule of tetrogen; that is why the data of this nitramine fulfill this correlation.

In the case of straight line D in Fig. 1, the $\Delta H_{m,tr}$ values increase in the order of CPX–tetrogen–HOMO [16]; this fact could be connected with the increasing hardness of their crystals in the mentioned sense. However, the hardness of these three compounds is not known—visually, the CPX crystals resemble a waxy (soft) substance. A part of data of straight line H in Fig. 2 can be viewed as a dataset of building blocks of the HNIW molecule (except for RDX, the skeletons of CPX and HOMO are components of the globular skeleton of HNIW). The structure of RDX can be obtained by notional introduction of a nitramino group into the CPX molecule or by a removal of methylene group from the HOMO molecule. Of course, it is interesting to compare the sensitivity of substances involved in the two straight lines with the lengths of the N–N bonds that are first split in their molecules during initiation (see Zeman and Jalový [27] and references therein): these bond lengths increase in the order of CPX (0.1346 nm)–tetrogen (0.1355 nm)–HOMO (0.1377 nm in its position 1)–RDX (0.1398 nm)–ε-HNIW (0.1436 nm in its position 2). For the first three members of this series, the bond lengths were calculated (see Zeman and Jalový [27] and references therein), and it can be seen that their order agrees with the sensitivity order; substances RDX and especially ε-HNIW exhibit a distinct stabilizing effect of crystal lattice (compare the $\Delta H_{m,tr}$ values of all these nitramines); hence, the trend in N–N bond lengths is not completely concordant here with the calculated *BDE* values.

Application of the approach described by Fried et al. [3] and modified by Song et al. [4] to the study performed in this present work has led to Figs. 3 and 4. No simplification was achieved. The straight lines with positive slopes have a logical course, which is usual in the case of the solid lines adopting the BDE/E_{total} ratios; increasing energy content of the molecules

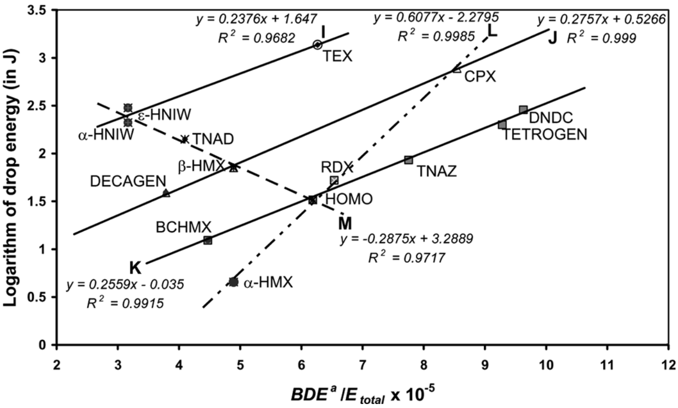


Figure 3. Semi-logarithmic relationship between the BDE^a/E_{total} ratio, obtained by UB3LYP/6-31G* method, and impact sensitivity (expressed as drop energy) of the studied nitramines.

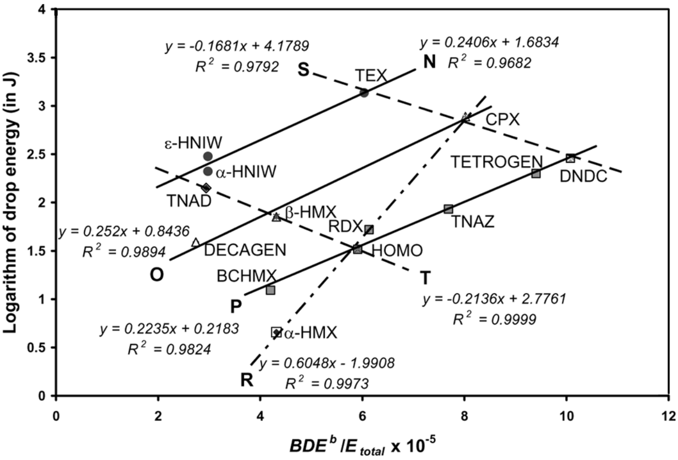


Figure 4. Semi-logarithmic relationship between the BDE^a/E_{total} ratio, obtained by UB3LYP/6-31+G* // PM3 method, and impact sensitivity (expressed as drop energy) of the studied nitramines.

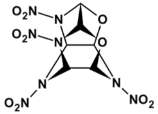
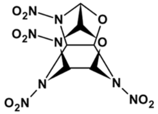
of these nitramines involved in these straight lines corresponds with increasing impact sensitivity. However, in our earlier paper [28] we proved that a specific feature of several nitramines is the decrease in their impact sensitivity connected with increase in their performance in the order of RDX–HMX–TNAZ–α-HNIW–ε-HNIW. This fact is also partially seen in Figs. 3 and 4, especially in straight lines M and T. This could perhaps be connected with the consonant influence of the intensity of intermolecular forces and that of the lengths of N–N bonds that are first split in the respective crystals, in analogy with the situation mentioned in the case of straight lines D and H in Figs. 1 and 2. A similar consideration could also be true of straight line S in Fig. 4 if we take into account the distinct similarity of the molecular structures (relationships between the imidazoline and piperazine skeletons); no analogy of such dependence is present in Fig. 3. As for straight line L in Fig. 3 and straight line R in Fig. 4, both of them correspond to notional deriving of the α-HMX structure from the CPX structure, and their courses are logical.

In contrast to Figs. 1 and 2, the application of BDE/E_{total} has included all the experimental values of drop energies from Table 1 in the correlations given in Figs. 3 and 4. In this case, particularly the UB3LYP/6-31+G* // PM3 (UHF) method provides relationships of better quality compared with the application of the BDE values alone. It is mainly the consequence of the interactions in the real molecular crystal (and hence also real conformation of the molecule) that it is impossible to achieve a simplified relationship between the impact sensitivity and the BDE/E_{total} ratios—such a relationship as that considered by Fried et al. [3] and Song et al. [4]. In addition, Fried et al. [3] attempt to compare (in this way) substances characterized by various mechanisms of primary fission within the initiation process.

One of the contemporary aims of research on energetic materials is focused on syntheses of the polycyclic nitramines 4,8,10,12-tetranitro-2,6-dioxa-4,8,10,12-tetraazaisowurtzitane (Aurora-5 or TNIW-5) and 4,6,10,12-tetranitro-2,8-dioxa-4,6,10,12-tetraazaisowurtzitane (Aurora-6 or TNIW-6) [29]

Table 3

A survey of the predicted drop energies, E_{dr}, for TNIW

Data no.[a]	Nitramine	Predicted impact sensitivity by means of Fig.	line	E_{dr} in J	Averaged E_{dr}value in J	Structural formula
12	TNIW-5	1	A	10.45	12.54 ± 2.78	
		2	G	10.93		
		3	I	13.16		
		4	N	15.63		
13	TNIW-6	1	A	10.66	12.16 ± 1.62	
		2	G	10.42		
		3	I	13.21		
		4	N	14.38		

[a] Numbering according to Table 1.

(for their structural formulas, see Table 3). If the relationships found in Figs. 1–4 are applied to predicting the impact sensitivity of these intramines, then the results summarized in Table 3 are obtained. This survey documents a relatively large difference between the approaches in the sense of Figs. 1–2 and those in the sense of Figs. 3–4. Hence, the resulting average values are loaded with a larger error; nevertheless, they correspond to the expectations.

Conclusions

The well-known semi-logarithmic relationship between the calculated bond dissociation energies, *BDE*s, and the impact sensitivity is not unambiguous, not even in the case of identical mechanisms of primary fission within the initiation process (the homolysis of N–N bond in this case). Its derivation can be speculative to a certain extent. In contrast to the published data [3,4], the replacement of the *BDE* values by their ratios to total energy, E_{total}, of the molecule (i.e., by BDE/E_{total}) does not lead to any simplification of the said relationship. However, this operation markedly increases the quality of the partial relationships found; in this respect, the UB3LYP/6-31+G* // PM3 method gave results of higher quality as compared with those obtained by means of the UB3LYP/6-31G* approach. The ambiguity of the relationships found is mainly due to the real conformation of the molecules and the intermolecular force effects within the real molecular crystals, which are involved in neither of the two calculation methods (their results concern isolated molecules), but they play a very significant part in the real impact sensitivity of energetic materials [1,7,15,16,23,26]. The more detailed analysis of results obtained in our case from a larger set of polynitro compounds of a single kind is the reason why our results differ from those published earlier [3,4].

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some standards in Table 1 and for several impact sensitivity measurements.

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