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Sensitivity of energetic materials: Evidence of thermodynamic factor on a  large array of CHNOFCl compounds

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A R T I C L E I N F O

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A B S T R A C T

Mechanical and thermal hazards are critical for chemical compounds. Foremost, the design of novel energetic materials that are stable, insensitive, but have a detonation performance superior to in-service materials is of great interest. However, a single source of safety data for hazardous materials with explosophoric functionalities is still missing. Herein, an experimental database on thermal stability, impact, and friction sensitivity for 150 CHNOFCl compounds is presented. Mechanical sensitivity is discussed in detail: particle size and shape effects, instrument design, and experimental protocol are considered. The entire dataset was analyzed using the simple descriptors of molecular structure. Mechanical sensitivity was found to be linearly correlated with the maximal heat of explosion for certain classes of compounds (nitrobenzenes, furazans, pyrazoles, etc.). Consideration of all species shows that previously proposed sensitivity increase with an energy content rise is relevant, although it is

not strict line, as was assumed, but rather a widened “strip”. A new parameter, safety factor, is proposed to

combine two types of sensitivity data. With this factor, the limiting values of mechanical sensitivity at a given energy content are provided that represent the state-of-art development of energetic materials and may be used for screening and design of novel compounds.

# Introduction

Current developments in the field of high-energy density materials are associated with efforts to create target compounds with high energy content and improved safety (reduced sensitivity toward external stimuli). Thus, the response to thermal and mechanical stimulus is one of the most important functional parameters of energetic materials. How-

ever, the problem of understanding of the origins of material’s sensi- tivity and its correlations with some structural parameters, mostly

studied in literature and present study for energetic compounds, is supposed to have much broader applicability to other hazardous mate- rials. Indeed, the energetic materials are based on organic frameworks (benzene, imidazole, pyrazole, tetrazole, furazan, furoxan), and include the explosophoric functionalities (e.g., nitro-, azo- groups), the struc- tural features that can be found in various chemicals (drugs, radical initiators, etc). However, even with an increased capability of compu- tational chemistry [[1,2]](#_bookmark38), in most cases the parameters of a target

compound are determined experimentally, and synthetic efforts repre- sent a trial-and-error process. Some examples of the prediction of the key properties of energetic materials to guide chemists emerged recently [[3,4]](#_bookmark39), but are still in the infantry stage.

An important aspect of any prediction approach is the *data*, that should refer to the samples with a wide range of molecular fragments and provide reliable values of the target quantities. With regard to the safety properties of energetic materials, several datasets had been re- ported to date, which, however, have a limited set of molecules and are assembled from chemically similar compounds. This forces researchers to use the experimental data from various sources when performing theoretical analysis. However it is known that the sensitivity indicators obtained by different methods should be compared at least with a great

caution (e.g., [[5–7]](#_bookmark40)). Below we will briefly discuss the available sets of sensitivity data, focusing on the implications of those results for the

general performance-sensitivity problem of energetic materials.

The first hypotheses about the nature of the structure-sensitivity

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relationship for energetic materials dates back to 19th century. Berthelot

*MW*

1000(28.9(*NH* — *NF* ) + 94*NC* + 64.8*NF* + Δ*H*0 )

suggested that the sensitivity is directly related to a thermodynamic

quantity, namely, the heat of detonation, and, as further discussion and

*Qmax* =

*f* , *α* > 1 (3)

our results will show, these parameters do indeed correlate well [[8]](#_bookmark43).

Vant-Hoff noticed that there are some structural moieties that reveal the higher instability (explosophoric functionality) of certain compounds [[8]](#_bookmark43). Since about the 1930 s, reliable instruments for determining me- chanical sensitivity have become available, and the first comparative studies of the sensitivity of related chemical structures have been pub- lished. Thus, Kholevo [[9]](#_bookmark44) and independently Wo¨hler and Wenzelberg

[[10]](#_bookmark45) based on the study of four alkyl-derivatives of trinitrobenzene, showed that mechanical sensitivity increases with an increase in the number of methyl groups.

In their seminal papers, Kamlet and Adolph significantly expanded the list of considered compounds and reported the impact sensitivities for 33 nitroaliphatic [[11]](#_bookmark46) and 38 nitroaromatic explosives [[12]](#_bookmark47). They used the Explosive Research Laboratory (ERL) impact machine with type 12 tools, where the determined impact sensitivity is expressed as a drop height resulting in 50% of explosion, *H*50 [cm]. When they narrowed

down the sample, examining only nitroaromatic explosives with an α-C –

H bond, impact sensitivity was found to be linearly correlated with the

proposed measure of the oxygen balance of these compounds, taken as:

where the oxygen coefficient is defined as *α* = *N*O / [2*N*C – (*N*H – *N*F)/

2]. The *Q*max parameter assumes the full conversion of CHNOF material to HF, H2O, N2, and CO2 products, which is much similar to the maximal heat of explosion alternatively proposed by Kamlet [[26]](#_bookmark60). Below we will

refer the correlations of *Pcr* data with *Q*max values as the “energy- sensitivity rule”, which, according to Pepekin et al., is a linear rela-

tionship. This relationship, derived from the analysis of 13 energetic

materials, indicates the impossibility of creating more powerful and, at the same time, safer compounds. Thus, the authors postulate “the limited capabilities of organic explosives” [[22]](#_bookmark56).

The impact sensitivity for a set of 23 explosives and 23 mixtures

thereof was determined by Licht [[27]](#_bookmark61) using the BAM machine and represents the drop weight *W* [N∙m] at which one of the six tested samples explodes. This study also supports an increase of sensitivity with

the energy content growth. However, Licht pointed out three outliers from general trend, viz., triaminotrinitrobenzene (TATB), 2,6-diamino- 3,5-dinitropyridine-N-oxide and HMX/TNT mixture. That is, some interesting results can be expected for low-sensitive explosives. For mixed explosive compositions, non-additive effects can be realized.

*OB*100 = 100(2*NO* — *NH* — 2*NC* — 2*NCOO*)

*MW*

(1)

Recently, Smirnov et al. [[28]](#_bookmark62) reported the compilation of impact and friction sensitivity data for 31 individual energetic material. These

where *N*C, *N*H, *N*O, - are the numbers of carbon, hydrogen, and ox- ygen atoms, respectively, and *N*COO is the number of carboxyl groups in the molecular formula, and *MW* is the molar mass of the molecule. Later, more rigorous statistical examinations proved the *OB*100 to be the most important descriptor within this dataset, even when various structural parameters from quantum chemical computations were also considered [[13]](#_bookmark48). Wilson et al. [[14]](#_bookmark49) reported the impact sensitivities of 40 aromatic compounds, some of which had more substituents than in the Kamlet report, and showed the correlation between impact sensitivity and *OB*100 parameter.

Storm et al. [[15]](#_bookmark50) collected data on impact sensitivity from various sources, obtaining a dataset of 258 compounds, including aromatic and heterocyclic nitro derivatives. Sensitivity, according to Storm, is re- flected by the sensitivity index (*SI*), which is described by the following correlation equation [(1)](#_bookmark4):

values were determined according to Russian standards [[29,30]](#_bookmark63). Impact sensitivity is represented by the frequency of explosions under constant drop energy level determined with two types of devices, *A*d1 and *A*d2 [%], respectively. Friction sensitivity values include the lower limit of pressure at which no explosion occurs within the test series, *P*LL [MPa]. All measured data were used by Smirnov et al. [[28]](#_bookmark62) to derive the regression equations for prediction of each safety parameter, e.g.:

*PLL* = 0.1(*ρQmax* )1.699 *α*—1.013 (500 — *Tm* )1.351 (4)

where ρ – density, *Q*max is the maximal heat of explosion defined by Eq. [(3)](#_bookmark3), α is the oxygen coefficient, and *T*m is melting temperature. As

can be seen, Equation [(4)](#_bookmark5) absorbs the previously proposed descriptors: the oxygen coefficient is used in line with Kamlet and Storm equations, and the heat of explosion as suggested by Pepekin.

A theoretical approach based on the molecular descriptors – sensi- tivity relationship was initiated by Politzer and Murray [[31,32]](#_bookmark64) and later

*SI* 100(*NO* — *NC* — *NH* /2 — *NCOO*) 5(*NC* + *NH* + *NN* + *NO*)

=

(2)

developed by Rice [[33]](#_bookmark65) and others [[34–36]](#_bookmark66). Correlations of this type use more complex parameters than previously considered *OB*100 or *Q*max,

Correlation approaches were further developed by Zeman group. Thus, correlations between sensitivity and thermal reactivity [[16]](#_bookmark51), thermochemical properties, structural parameters, or detonation per- formance [[17,18]](#_bookmark52) have been established for some classes of energetic materials.

Soviet and Russian researchers made important contributions to the development of the experimental methods of the impact sensitivity

testing [[7,19–21]](#_bookmark42). One of the most important results was the develop- ment of an advanced experimental technique, where deformation of a

thin layer of the unconfined pressed explosive has been observed and the impact sensitivity was expressed as the critical pressure of explosion initiation, *P*cr [GPa]. Pepekin and coworkers analyzed the available impact sensitivity data for common and novel energetic materials

[[20,22–24]](#_bookmark54) and found an almost linear increase of the impact sensitivity with the energy content growth [[22]](#_bookmark56). The latter thermodynamic quan-

tity was expressed using the maximal possible heat of explosion for this individual explosive, calculated according to [[25]](#_bookmark59):

1000(64.8*NF* — 28.9(*NH* — *NF* ) + 47[*NO* — (*NH* — *NF* )/2 ] + Δ*H*0 )

and require quantum chemical computations. The effectiveness of this technique has been tested on published datasets [[11,12,15]](#_bookmark46) containing mostly well-known energetic materials. The suitability of this approach for modern high-nitrogen compounds has yet to be demonstrated.

The larger the training set and the more diverse the compounds and measured properties included in it, the more accurate the predictive result can be expected. Obviously, a single source of reliable thermal, impact, and friction sensitivity data is highly needed. This dataset should contain the characteristics of both conventional and emerging energetic materials with a wide variety of structural units and groups. Here, the results of the Energetic Materials Laboratory of Semenov Federal Research Center for Chemical Physics, for several years are summarized. Note that some of the data that will be discussed in this report on the sensitivity and thermal stability of new compounds were mentioned in studies devoted to their synthesis, and were previously

scattered over different papers [[37–58]](#_bookmark67). Summarizing the data for new

and retested conventional energetic materials, the proposed dataset now includes the safety properties of 150 CHNOFCl compounds. All data

obtained using reliable standard procedures in uniform conditions. This

*Qmax* =

≤ 1

*f* , *α*

*MW*

dataset allows comparison of the importance of previously proposed

structural descriptors for sensitivity properties and assess the validity of the general correlation known as the “energy-sensitivity rule”. We infer that the presented data will be useful for development of the

computational approaches for predicting the properties of hazardous materials.

# Experimental

Thermal stability was assessed by linear heating of the material at 5 K min—1 rate within a DSC apparatus (DSC 204 HP, Netzsch). Samples weighting 0.1–2 mg were placed in the aluminum crucibles crimped with pierced lids. The melting point (*MP*) has been determined as the

extrapolated onset temperature of the endothermic peak [[59]](#_bookmark85), that is the temperature at which the extension of the baseline intersect the tangent line to a DSC peak drawn at the inflection point. As a measure of thermal stability (*TS*), the extrapolated onset of the exothermic DSC peak was used. For samples that vaporize being heated in conventional runs at normal pressure, additional measurements were conducted at elevated pressure of 2.0 MPa. Further details of the pressure DSC technique applied to energetic materials can be found elsewhere [[43,60]](#_bookmark71).

Impact and friction sensitivities were determined according to STANAG standards [[61,62]](#_bookmark86) on BAM-type machines. Full series of ex-

periments include 25–30 trials with the powdered sample loaded with 40 mm3 (for impact) and 10 mm3 (for friction tests) spoons. The first

departure from the standard procedure was that during these explor- atory tests, the particle size of the samples was not controlled. As- synthesized powders were mostly finer than that specified by STANAG

4489 (0.5–1 mm), but conform STANAG 4487 (less than 0.5 mm). The respective raw data (“GO”/”NO-GO” at a stimulus level) was analyzed

using the Bruceton technique [[63]](#_bookmark87). The second departure of the adopted procedure over the standard protocol appears when the scatter of the results is high, i.e., the ratio of standard deviation of *H*50 to logarithmic step of drop heights *S*/*D* > 2 (a typical step *D* was 0.1). In this case, the additional tests were performed to give several levels with 10 results. Then, all bunch of data was analyzed by probit analysis [[64,65]](#_bookmark88). The output values correspond to the impact sensitivity (*IS*) as a drop energy *E*50 [J] that corresponds to 50% of explosions and the friction sensitivity (*FS*) is the friction force *F*50 [N] that initiates 50% of explosions.

# Results and discussion

Commonly used safety parameters. Safety parameters obtained in

small-scale tests, namely, thermal stability, impact and friction sensi- tivity, are currently the “golden standard” for preliminary hazard assessment of an energetic material [[66–69]](#_bookmark89).

The preliminary small-scale thermal stability characterization in-

cludes two thermal parameters – the melting point (*MP*) and the extrapolated onset of the decomposition event, an accepted measure of

thermal stability (referred as *TS* below). *TS* parameter has several ad- vantages including ease of interpretation, short measurement time, and good reproducibility (typically the deviation between *TS* values in

parallel runs is less than 5 ◦C). The problem is that using a single

characteristic, that strongly depends on the experimental conditions, we cannot clarify the entire (kinetic) picture of the thermal stability of the

material under study. For example, we have recently showed that for hydroxylammonium 5,5′-bistetrazole-1,1′-diolate (TKX-50) the initial data indicating its higher thermal stability than the reference RDX are

not confirmed. Detailed kinetic analysis reveals that the thermal sta- bility of TKX-50 is lower than that of RDX [[70]](#_bookmark92). Therefore, thermal stability analysis should include the determination of a complete set of kinetic parameters of thermal decomposition [[40,43]](#_bookmark70). However, even with the kinetic parameters in hand, the prediction of thermal behavior of compounds should be done with great care for temperatures far beyond the temperature range covered by the primary data [[71]](#_bookmark93). In view of the above, the melting point and the temperature of the onset of decomposition are convenient values for the *first* assessment of thermal stability.

For new energetic materials, the values of mechanical sensitivity are of practical interest, characterizing their response to shock and friction.

The experimental factors affecting the resulting sensitivity and various

measurement protocols have been extensively reviewed in the literature [[7,8,28,72–75]](#_bookmark42). A prerequisite remark before the ensuing discussion is that the term *sensitivity* will be used in the traditional way. In fact, it does

not represent the mechanical sensitivity of a specific explosive, but its

response to the specific loading conditions [[7,76]](#_bookmark42). Conceptually, the sensitivity is governed by factors from at least three levels: the “mo- lecular level” (chemical nature of the compound), the “powder level”

(particle size, particle shape, mechanical properties, etc.), and the “in- strument level” (assembly type, reaction criteria, relative humidity, etc.). While it is tempting to attribute the sensitivity exclusively to the

first level and use it as a constant of a chemical compound, the long experience tells us that the latter factors significantly contribute the resulting value. Thus, we can repeat after Kamlet and Adolph [[12]](#_bookmark47):

“since the impact machine has neither resolution nor the reproducibility required of a research tool, the work was done under constraint that only

limited reliability could be attributed to any individual result”.

A unique and problematic feature of the mechanical sensitivity tool, is that it cannot be calibrated, in the same way as, for example, a thermal analyzer is calibrated against the melting points of standard samples. The results obtained with various impact machines vary considerably, and even using the similar type of machine and the same experimental protocol, different results can easily be obtained (see e.g., [[77]](#_bookmark96), [Table 1](#_bookmark7)

and discussion below). Afanas’ev and Bobolev [[7]](#_bookmark42) formulated this intrinsic feature of sensitivity testing and put forward the so called

“pivotal row” of well-known energetic materials. They note that the long

experience of the practical work with energetic materials claims that the mechanical sensitivity increases in the following order: 2,4,6-Trinitro- toluene (TNT) > Picric acid > Tetryl Hexogen (RDX) Octogen (HMX) > Pentaerythritol tetranitrate (PETN) > Lead azide > Mercury fulminate. Therefore, the same relative order of sensitivity determined with the apparatus is a necessary (but not sufficient) condition of the reliability of the experimental technique. As can be seen by comparing the gray columns in [Table 1](#_bookmark7), all selected datasets from the literature and the results of this study pass this test. In fact, for five of these com- pounds, STANAG standards give typical results for a particular type of equipment [[61,62]](#_bookmark86). These benchmark values are complemented by the results of NATO Round robin test [[6,78]](#_bookmark41) (only impact sensitivity is

≥ ≥

given) and compared with our data: PETN – 5 J [[61]](#_bookmark86) (our result: 3.3 ±

0.3 J, NATO Round robin test: 4.1 ± 0.9 J [[6,78]](#_bookmark41)), RDX – 8 J (our result:

10.5 ± 2.5 J (average on 6 lots), NATO Round robin test: 10.6 ± 2.2 J [[6,78]](#_bookmark41)), HMX – 9 J (our result: 6.6 ± 2.6 J (most coarse powder, other results on [Fig. 2](#_bookmark11)), NATO Round robin test: 6.8 ± 1.7 J [[6,78]](#_bookmark41)), Tetryl – 17 J (this study: 14 ± 4 J, NATO Round robin test: 15.4 ± 3.1 J [[6,78]](#_bookmark41)), TNT – 30 J (this study: 30 ± 5 J, NATO Round robin test: 36 ± 6.5 J [[6,78]](#_bookmark41)); for friction sensitivity: PETN – 67 N (our result: 71 ± 10 N), RDX

– 133 N (130 ± 15 N), HMX – 113 N (130 ± 15 N), Tetryl > 353 N (205

± 20 N), TNT > 353 N (>360 N).

The extension of the “pivotal row” with some novel energetic com- pounds is not straightforward: the relative position of CL-20, FOX-7,

NTO, BTF as reported by various authors varies largely (see [Table 1](#_bookmark7)). In order to verify *our* experimental data, we compare the results of this study with the impact sensitivity data obtained earlier by Russian re- searchers These papers published the results of academic research based on rigorous experimental work, where the impact sensitivity is deter- mined as a critical pressure corresponding to 50% of explosions of thin pressed pellets in unconfined flow conditions. [Fig. 1](#_bookmark10)a shows that the

drop energy, *E*50, from this study is proportional to the square of critical pressure, *P*cr , for 18 compounds. That is, the *E*50 (*P*2cr) dependency is

linear, as it was theoretically proposed by Dubovik [[75]](#_bookmark95) using the drop energy and the critical pressures from the same experiment. However, here the high correlation of the impact sensitivity as the drop energy with a critical pressure obtained by completely different procedure is shown. In addition, the friction sensitivity of selected compounds is proportional to the critical pressures reported in literature ([Fig. 1](#_bookmark10)b). This observation is supported by a previous compilation by Afanas’ev and

**Table 1**

Impact and friction sensitivity for some common energetic materials: literature data and results of this study.

Parameter Method **Lead azide**

**ZOX PETN ε-CL-20 BTF ADN HMX RDX Tetryl FOX-7 Picric acid DINGU LLM-**

**105**

**TNT NTO NIGU**

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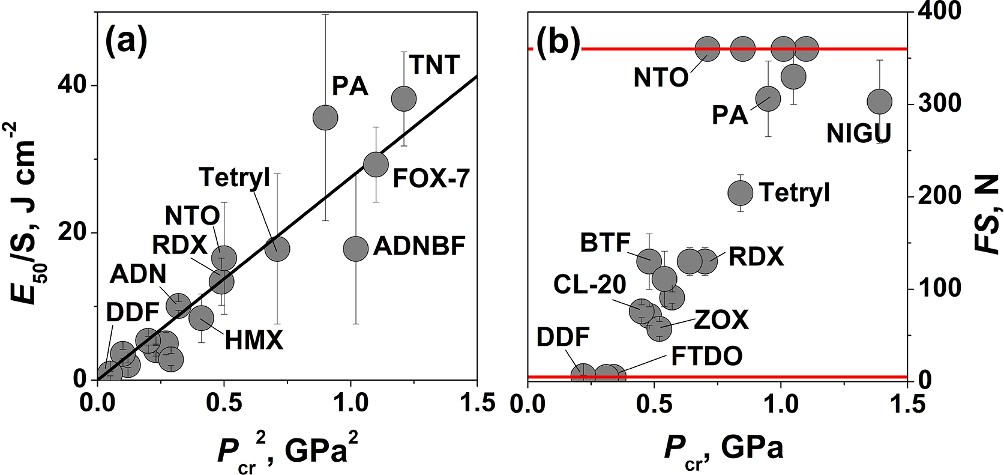
4

Notes: ZOX – 1,1,1,3,6,8,8,8-octanitro-3,6-diazaoctane, PETN – pentaerythritol tetranitrate, CL-20 – 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.03,11.05,9]dodecane, BTF – benzotrifuroxan, ADN – ammonium dinitramide, HMX, RDX – 1,3,5-trinitro-1,3,5-triazinane, Tetryl – 2,4,6-trinitrophenylmethylnitramine, FOX-7 – 2,2-dinitroethene-1,1-diamine, Picric acid – 2,4,6-trinitrophenol, DINGU – 1,4-dinitroglyco- luril, LLM-105 – 3-nitro-1,2,4-triazol-5-one, TNT – 2-Methyl-1,3,5-trinitrobenzene, NTO – 2,6-diamino-3,5-dinitropyrazine-1-oxide, NIGU – nitroguanidine.

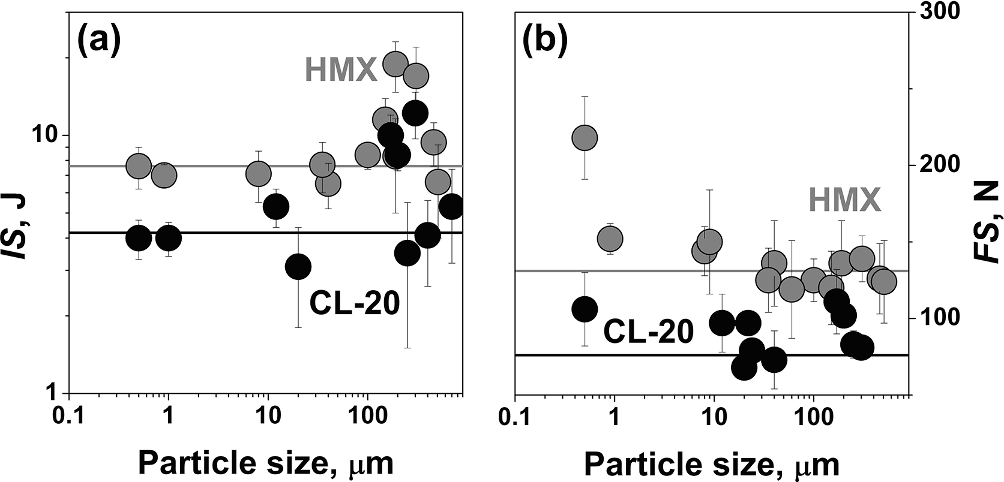
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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Impact** |  | | | | | | | | | | | | | | | | |
| *H*50, cm | ERL | 2–4 | 9 | 10–16 | 12–21 | 14–53 |  | 24–32 | 22–28 | 32–39 | 34–71 | 64–87 | 88–125 | 158 | 98–160 | >280 | >320 |
|  | machine, | [[12]](#_bookmark47) | [[99]](#_bookmark112) | [[12,100]](#_bookmark47) | [[100]](#_bookmark113) | [[14,101]](#_bookmark49) |  | [[12,100]](#_bookmark47) | [[12,101]](#_bookmark47) | [[12,101]](#_bookmark47) | [[85]](#_bookmark103) | [[12,14,102]](#_bookmark47) | [[103]](#_bookmark115) | [[104]](#_bookmark116) | [[12,14]](#_bookmark47) | [[87]](#_bookmark105) | [[101]](#_bookmark114) |
|  | type 12 |  |  |  |  |  |  |  |  |  |  |  |  | 70–80 |  | 291 |  |
|  | [[11]](#_bookmark46) |  |  |  |  |  |  |  |  |  |  |  |  | [[105]](#_bookmark117) |  | [[15]](#_bookmark50) |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  | 40–120 |  |  |  |
| *A*d1, % | K-44–2 |  | 100 | 100 [[28]](#_bookmark62) | 100 [[28]](#_bookmark62) | 92 [[28]](#_bookmark62) | 80–90 | 92 [[28]](#_bookmark62) | 80 [[28]](#_bookmark62) | 44–60 | 16 | 25–32 |  | 32 [[28]](#_bookmark62) | 4–9 | 8 [[28]](#_bookmark62) | 0 [[28]](#_bookmark62) |
|  | machine, |  | [[28]](#_bookmark62) |  |  |  | [[106]](#_bookmark118) |  |  | [[28,72]](#_bookmark62) | [[28]](#_bookmark62) | [[28,106]](#_bookmark62) |  |  | [[28,72]](#_bookmark62) |  |  |
|  | Device #1 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | [[28]](#_bookmark62) |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| *A*d2, % | K-44–2 | 100 | 100 | 100 [[28]](#_bookmark62) | 100 [[28]](#_bookmark62) | 96 [[28]](#_bookmark62) |  | 100 [[28]](#_bookmark62) | 92 [[28]](#_bookmark62) | 24 [[28]](#_bookmark62) | 72 | 0 [[28,106]](#_bookmark62) | 92 | 76 [[28]](#_bookmark62) | 0 [[28]](#_bookmark62) | 84 | 0 [[28]](#_bookmark62) |
|  | machine, | [[72]](#_bookmark94) | [[28]](#_bookmark62) |  |  |  |  |  |  |  | [[28]](#_bookmark62) |  | [[28,106]](#_bookmark62) |  |  | [[28]](#_bookmark62) |  |
|  | Device #2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | [[28]](#_bookmark62) |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| *P*cr, GPa | Confined | 0.18 | 0.52 | 0.66–0.74 | 0.37–0.45 | 0.56–0.65 |  | 0.71–0.88 | 0.80–0.95 | 0.80–1.25 | 1.05 |  |  |  | 1.06–1.40 |  | 1.38 |
|  | disc | [[20]](#_bookmark54) | [[20]](#_bookmark54) | [[20,24]](#_bookmark54) | [[24,107]](#_bookmark58) | [[20,23]](#_bookmark54) |  | [[20,23]](#_bookmark54) | [[20,23]](#_bookmark54) | [[20,24]](#_bookmark54) | [[23]](#_bookmark57) |  |  |  | [[20,23]](#_bookmark54) |  | [[24]](#_bookmark58) |
|  | disruption |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| *P*cr, GPa | K-44–2 | 0.26 |  | 0.49 [[21]](#_bookmark55) |  | 0.48 [[75]](#_bookmark95) | 0.57 | 0.62–0.73 | 0.7–0.78 | 0.84 [[21]](#_bookmark55) |  | 0.95 [[21]](#_bookmark55) |  |  | 1.07–1.20 | 0.71 |  |
|  | machine, | [[108]](#_bookmark119) |  |  |  |  | [[75]](#_bookmark95) | [[21,109]](#_bookmark55) | [[21,88]](#_bookmark55) |  |  |  |  |  | [[21,108]](#_bookmark55) | [[88]](#_bookmark106) |  |
|  | critical |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | height |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | method |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| *W*, N∙m | BAM | 4 | 3.6 | 2.5–3.5 | 4 [[111]](#_bookmark121) | 3.5 [[34]](#_bookmark66) | 3.7 | 4 [[27]](#_bookmark61)6.75 | 3.5–7.5 | 6.5–15 | 10 | 7.5 [[111]](#_bookmark121) | 5–6 |  | 15 [[27]](#_bookmark61) | 25 | >49 |
|  | machine, 1 | [[110]](#_bookmark120) | [[34]](#_bookmark66) | [[27,112]](#_bookmark61) | 1.7–4.3 |  | [[113]](#_bookmark123) | [[78]](#_bookmark97) | [[27]](#_bookmark61) | [[27]](#_bookmark61) 3 | [[112]](#_bookmark122) |  | [[111]](#_bookmark121) |  |  | [[27]](#_bookmark61)> | [[63]](#_bookmark87) |
|  | of 6 test | 7.5 |  |  | [[34]](#_bookmark66) |  |  |  |  | [[111]](#_bookmark121) | 20–40 |  |  |  |  | 120 |  |
| *E*50, J | This study | [[111]](#_bookmark121)  – | 4 | 3 | 4 a | 3 a | 8 | 7 a | 10 a | 14 | [[111]](#_bookmark121)  23b | 28 | 8 | 20 | 30 | [[63]](#_bookmark87)  13 a | >100 |
| **Friction** |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| *P*LL, MPa | K-44–3 |  | 100 | 100–175 | 60–150 | 100–150 | 300 | 200 [[28]](#_bookmark62) | 270 [[28]](#_bookmark62) | 350–400 | 330 | 450 [[106]](#_bookmark118) | 300 [[28]](#_bookmark62) | 400 | 600 [[28]](#_bookmark62) | 400 | 1150 |
|  | machine |  | [[28]](#_bookmark62) | [[106]](#_bookmark118) | [[99,106]](#_bookmark112) | [[99,106]](#_bookmark112) | [[106]](#_bookmark118) |  |  | [[28]](#_bookmark62) | [[28]](#_bookmark62) |  |  | [[28]](#_bookmark62) |  | [[28]](#_bookmark62) | [[28]](#_bookmark62) |
| *F*50, N | This study |  | 60 | 70 | 80 a | 130 a | 90 | 130 a | 130 a | 200 | 310b | 310 | 210 | >360 | >360 | ≈360a | 290 |

a The average value recorded in ten trials is given.

b See [Fig. 4](#_bookmark13) and the discussion therein.



**Fig. 1.** Impact (a) and friction (b) sensitivity data from the this study compared to literature data obtained using the critical pressure method [[7,20,75]](#_bookmark42). For impact sensitivity, a linear correlation is established between the parameters obtained by different techniques. On the plot (b), the red lines illustrate the lower and upper limits of the friction tester applied (5 and 360 N, respectively). The short names of compounds are disclosed in [Table 2](#_bookmark16). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



**Fig. 2.** Dependency of the impact (a) and friction (b) sensitivity of various lots of HMX (gray circles) and CL-20 (black circles) on the average particle size. The average sensitivity values of the most sensitive samples are shown as horizontal lines of the corresponding color.

Bobolev [[7]](#_bookmark42), which showed a parallelism in the critical pressures pro- voking an explosion under impact and friction. At present, it can be stated that the experimental techniques for measuring the sensitivity to impact and friction are validated and suggests that the results are reliable.

Above, we noted the wide spread of published sensitivity values for some new energetic compounds, as shown in [Table 1](#_bookmark7). What are the possible sources of discrepancies in literature data? First, the particle size and shape of the analyzed powder could affect the measured sensitivity. To give a baseline for this effect, we will consider a widely used nitramine explosive, HMX. Eleven lots of HMX were analyzed, from two submicron powders produced by cryochemical synthesis [[79]](#_bookmark98) and spray drying [[80]](#_bookmark99) to a coarse commercial with an average size of 500

μm. [Fig. 2](#_bookmark11) demonstrates the change in the level of sensitivity to impact

(a) and friction (b) for HMX, depending on the average size of the

fraction of the tested sample. In agreement with the previous studies by

Zeman [[81]](#_bookmark100) and Song [[82]](#_bookmark101), friction sensitivity of the nitramine de- creases with the particle size below 1 μm. However, the reason for the reduced friction sensitivity for submicron powder may be an artifact of

the method previously discussed by Radacsi et al. [[83]](#_bookmark102). In fact, when

tested with a BAM friction machine, a powder sample is poured onto ceramic plates with a roughness of 5–20 μm. The authors [[83]](#_bookmark102) supposed that the nanopowder could fill the grooves of the plate, thus without experiencing friction and exhibiting “virtual” insensitivity to it. Here, this effect hasn’t been studied in detail, as we focused on the larger

fractions, by measuring micron-sized samples following a standard

procedure. Friction sensitivity test results for another nitramine, hex- anitrohexaazaisowurtzitane CL-20, do not show a noticeable effect of in

the same range of particle size ([Fig. 1](#_bookmark10)b). Therefore, the observed decrease of friction sensitivity for nanosized HMX cannot be explained by the instrumental effect only, possibly a change of the polymorph phase and the hierarchical morphology of these powders also have an effect (e.g., [[79,84]](#_bookmark98)).

The character of changes in impact sensitivity depending on the size of HMX particles is more complex (see [Fig. 2](#_bookmark11)a). It is important to note that the fine powders and the powder with the largest particles (the only one that fulfills the STANAG 4489 requirement on particle size) all have the same impact sensitivity of 7.6 0.6 J (average value of these 9 samples).

±

As a possible reason for the maximum on impact sensitivity curve we infer some effects of the sample mass (note, that in these tests we back out of the standard). [Fig. 3](#_bookmark12)a demonstrates the changes in the explosion probability at a constant drop energy of 10.3 J for two different lots of

HMX. A curve for micron-sized powder having 100 µm particles has a characteristic hill-like shape, as is typically observed [[7,75]](#_bookmark42) for uncon-

fined pressed pellets. In our experiments, the situation is complicated by the additional compression of the loose sample upon impact and the obvious influence of the confinement. However, in principle, we observe the same transition from sample breakage to explosion at a certain critical mass. Registration of the drop rebound height in the absence of an explosion shows that the maximum of explosion probability corre- sponds to the minimal height value (not shown). Thus, the maximum of

the drop energy is absorbed at this point. Dashed rectangles depict the scatter of the sample masses that are taken with a 40 mm3 spoon by a

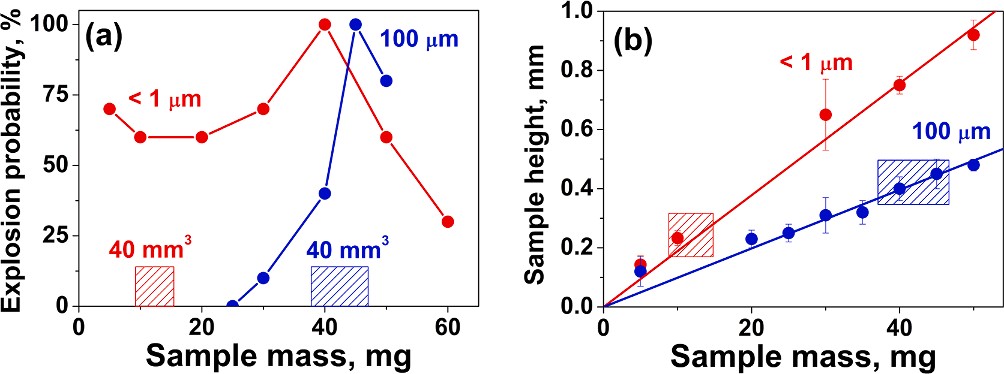
trained operator. As distinct from the micron-sized powders, taking of the same *volume* of sample, one obtains a much lower *mass* of the sample. [Fig. 3](#_bookmark12)b gives the height of the loose sample held by two rollers as a function of the sample mass. This height expectedly decreases with the sample mass, but the linear trend slows down when height approaches the average particle size of powder (see the lowest blue circle out of the linear fit, [Fig. 3](#_bookmark12)b). For an ultrafine HMX, the probability curve has a more complex shape with a local maximum near 5 mg, and another peak at 40 mg. Clearly, the layer of the sample in the analyzed range of masses is thicker that the single particle size. Thus, at this point it can be hy- pothesized, that the lower maximum of explosion probability corre- sponds to the primary breakage of the sample, while the maximum at 40

mg – to the secondary breakage [[75]](#_bookmark95). The effect of the particle size has to be studied further. Note however, that the standard procedure where the

volume of the sample is fixed and Bruceton statistics is applied, “blurs”

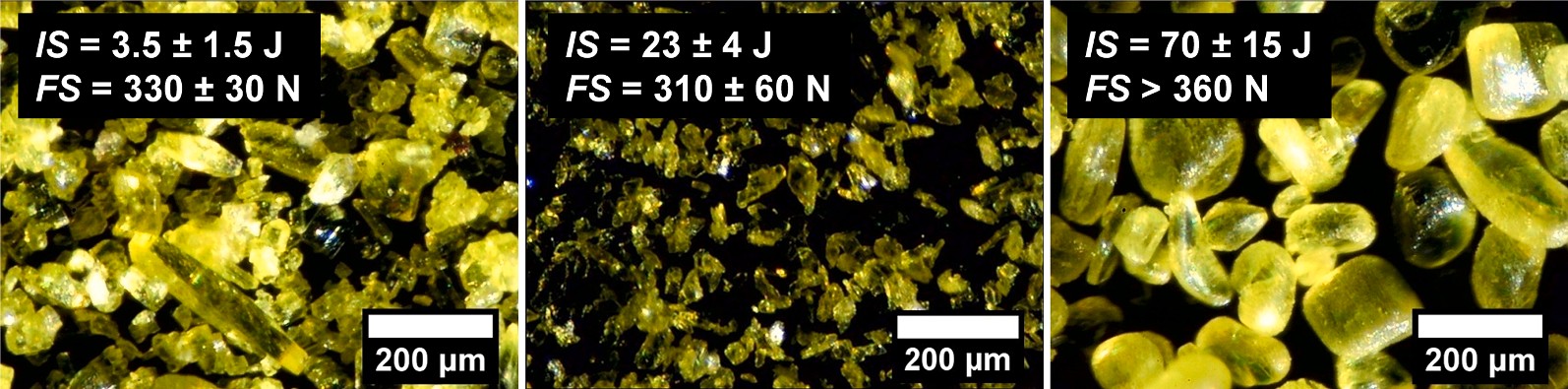
the difference between submicron and micron-sized lots of HMX and gives the same impact sensitivity within the errors (e.g., [Fig. 2](#_bookmark11)a).

A clearer dependence of the sensitivity to mechanical stress on the size and type of particles is observed for 2,2-dinitroethene-1,1-diamine (FOX-7). A similar trend is probably typical for low-sensitivity ener- getic materials with a high melting point (*vide infra*). [Fig. 4](#_bookmark13) demonstrates the differences in the morphology of the investigated lots of FOX-7 and their sensitivity determined in this study. Tuning the particles morphology changes the impact sensitivity drastically, i.e., from 3.5 to



**Fig. 3.** Dependence of the explosion probability (a) and the sample height (b) on the sample mass for two lots of HMX. The average particle size for a specific powder is shown next to the curve. Dashed rectangles illustrate the mass range reached with a 40 mm3 spoon. The value indicated by each dot is the average of

10 tests.



**Fig. 4.** Morphology and impact sensitivity values for three lots of FOX-7. The impact and friction sensitivity obtained for these powders are shown in the insets.

70 J, which qualitatively agrees with the literature reports. Thus, Sleadd et al. comparing FOX-7 powders of different particle size and shape, noted some variation of the impact sensitivity values [[85]](#_bookmark103) . Khvorov et al. using the critical thickness of the detonating layer technique, re- ported the FOX-7 sensitivity ranging from high to low [[86]](#_bookmark104). Elucidation of the influence of various factors on the impact sensitivity of the FOX-7 requires additional special studies. However, for the further analysis of

the structure–property relationship, we have chosen a value of 23 ± 4 J,

that agrees well with the Afanas’ev data for FOX-7 ([Fig. 1](#_bookmark10)a), and qual- itatively agrees with the friction sensitivity results. Another outcome of

the results for FOX-7 is that the friction sensitivities are much less disturbed by the powder properties for high-melting energetic materials. For other compounds from this group, we cannot catch the particle morphology effects since only single lot or two lots were analyzed in this study, but it can be supposed because of the considerable span within the reported in literature sensitivity data. Thus, nitrotriazolone (NTO) is generally classified as an impact insensitive explosive, for which the impact sensitivity is illustrated by the high drop heights > 280 [[87]](#_bookmark105) or 291 cm [[15]](#_bookmark50), However, Dubovik showed that the critical pressure of

explosion for NTO is 0.71 GPa [[88]](#_bookmark106), that is at the RDX level (0.7–0.8

GPa, [Table 1](#_bookmark7)). In an earlier report, NTO sensitivity was quoted as 22 J [[89]](#_bookmark107), indicating moderate sensitivity; however, the experimental method and other details were not specified. Recently, Delage et al. [[90]](#_bookmark108) reported the impact sensitivity of NTO powders with different particle

size distributions. So, for ~ 300 μm particles, the sensitivity was 18–19 J, for ~ 50 μm particles 9–11 J, and at ~ 12 μm it was 8–13 J. That is,

—

the impact sensitivity increases with decreasing particle size, while all these batches are insensitive toward friction (friction sensitivity above 353 N). The value of 13 6 J obtained by us for powders with non- optimized particle size distribution and shape is consistent with most of the literature data and can be recommended as a conservative esti- mate of impact sensitivity for NTO. The reported impact sensitivity data

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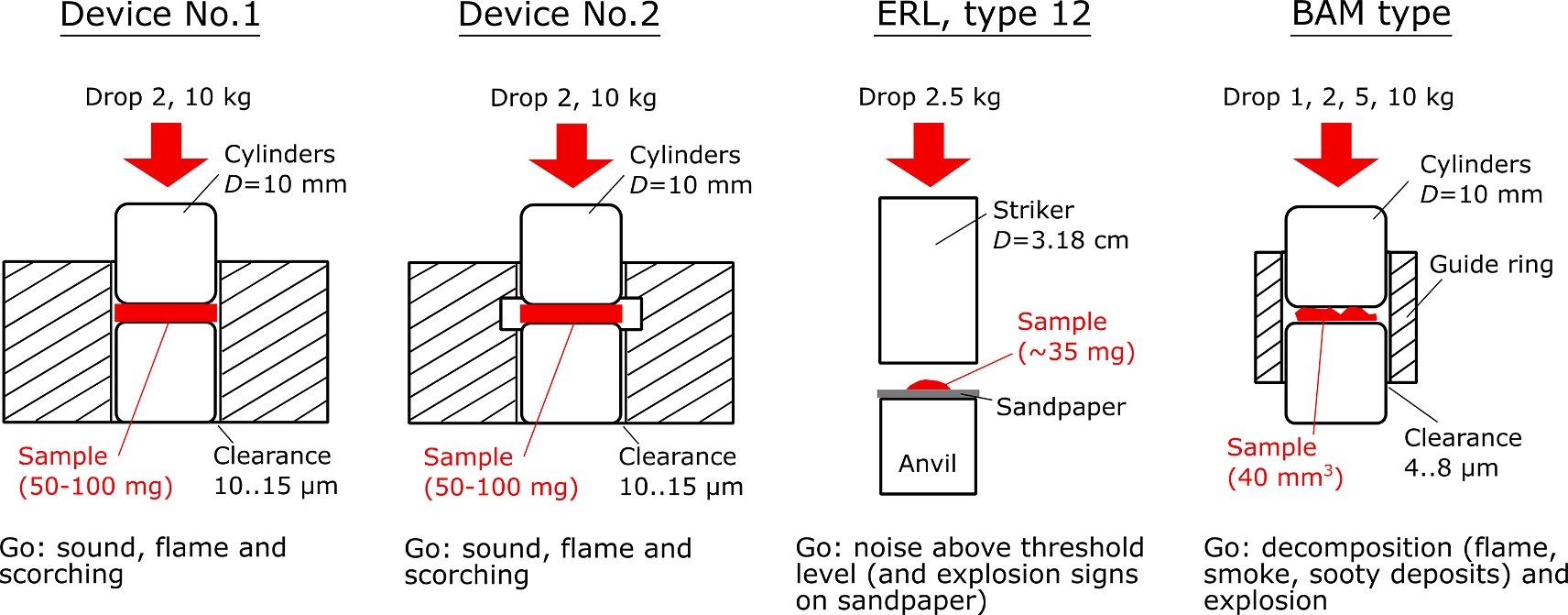
for LLM-105 (2,6-diamino-3,5-dinitropyrazine-1-oxide) differ signifi- cantly; the value of 40 cm or 120 cm is given by different authors [[91,92]](#_bookmark109). The impact sensitivity measured in this study is 20 J, that qualitatively the sensitivity ranking from literature.

Few types of impact machines are known for determining the impact sensitivity of energetic compounds. The most significant differences in the assembly design of the currently used impact machines are shown in [Fig. 5](#_bookmark14). The present study was carried out using a BAM-type device. Its important design feature is the clearance (gap) between the guide ring and the rollers, i.e., the sample flow is retarded. As it was shown by Soviet researchers [[93,94]](#_bookmark110), the flow conditions largely affect the measured sensitivity. Thus, when the clearance between the rollers and the guide ring was reduced to zero, some explosives were not exploding at high drop energies. At the same time, in the so-called device No.2 ([Fig. 5](#_bookmark14)), where the groove facilitates the free-flowing conditions of the impacted sample, the same compounds reveal explosions. Based on these results, Kholevo [[8]](#_bookmark43) concluded that the *flow* (fast inelastic defor- mation) is a prerequisite for the initiation of explosion. Indeed, the re- sults collected by Smirnov[[28]](#_bookmark62) show that the energetic materials for which we noted the spread between the values given by different au-

thors – high-melting explosives with high mechanical strength – these

compounds (e.g., LLM-105, NTO, FOX-7 in [Table 1](#_bookmark7)) show a lower per- centage of explosions in test with confined sample (so-called device No.1, [Fig. 5](#_bookmark14)) compared to free-flowing conditions (device No.2, [Fig. 5](#_bookmark14)). Overall, the assembly design and flow conditions are considered as very strong factors affecting the measured sensitivity.

A third factor that clearly influences the determined impact sensi- tivity is the criteria applied for judging whether the measurement result was positive. [Table 1](#_bookmark7) lists the Kamlet results obtained with the ERL machine, when a positive event was judged only by a noise level above the certain threshold [[26]](#_bookmark60). Note that the recent STANAG 4489 standard for ERL-type machine specifies that both sound criteria *and* explosion



**Fig. 5.** Comparison of the several assembly designs, used in standard procedures. From left to right, the core assembly units are shown used in K-44–2 impact machine (Kuibyshev Polytechnic Institute) called device no. 1 with chamfered rollers and device no.2, ERL (Explosives Research Laboratory) impact machine with

type 12 tools, BAM (Bundesanstalt für Materialforschung) impact machine. Below the assembly scheme, the criteria for positive event specified in the respective standard are shown.

signs on the sandpaper should appear. However, the results in the first row of [Table 1](#_bookmark7) are mainly determined based on sound criteria only. On the other hand, our results, according to the STANAG 4489 standard, include *both* decomposition and explosion as a positive event. For compounds that decompose without sound effect, a lower impact sensitivity is obviously recorded. Several researchers have encountered this phenomenon. Mullenger determined the limiting energy of *explosion* and the limiting energy of *decomposition* [[6]](#_bookmark41). While the explosion

occurred only for “classical” explosives such as lead azide and RDX, a

decomposition reaction took place for less powerful PBX-type and py- rotechnic compositions. Zeman discussed the impact sensitivity deter-

mined using the “first reaction” criteria (not specified in paper) as compared to the sound criteria [[18,95]](#_bookmark53). The value of the first indicator

(apparently corresponding to the decomposition criterion) is always significantly less than the second (corresponding to the sound criterion) for insensitive explosives. For example, for DINGU the first value is 5.6 J,

while the second parameter is – 24.6 J, for NTO – 15.9 versus 71.6 J, for NIGU – 9.2 versus 45.5 J. It has been shown that for “classical” com-

pounds from the so-called benchmark series (TNT, HMX, RDX and others), the difference between these two values of impact sensitivity is insignificant.

From the above summary, we can conclude that the mechanical sensitivity of a compound is a very specific value, measured using a very

specific “ruler”. Compliance with a standard protocol, years of experi- ence, consideration of different batches of material and broad compar-

ison with reference compounds and literature seems to be the only way to obtain reliable results. To compare the sensitivity of materials, it is necessary to take values from one source. At the same time, further analysis should take into account the low resolution of the technique

(“rulers”).

Next, we will try to identify the correlation between the chemical structure of an energetic material and the parameters of its temperature

and/or mechanical sensitivity. In this discussion, as opposed to “normal” energetic materials (let’s call them *group I*), compounds with reduced energy content (*group II*) and expected low sensitivity (*group III*) will be

considered. Group I comprises the most of investigated energetic ma- terials, and the idea behind introduction of the other two groups is to locate the compounds with above discussed critical factors (flow, decomposition instead of explosion under impact, positive event criteria). To fall into group II, a compound must meet one of the

following criteria: (*i*) the calculated maximum heat of explosion, Qmax, is less than 1000 cal g—1, (*ii*) no exothermic decomposition is observed in

the DSC even at elevated pressure, or (*iii*) the maximum limit set for the impact sensitivity machine are achieved (namely, at 100 J, less than 50% of explosions occur). In the subset of low-sensitive and high- melting compounds (group III), we select the materials for which no melting point is registered by DSC and whose friction sensitivity is

higher than the typical nitramine level (150 N). Note, that the larger- scale experiments, like on the detonation spreading on the environ- mental mass of the explosive [[20,86]](#_bookmark54) and the critical thickness of the detonation-capable layer [[20,86,96]](#_bookmark54) show that compounds falling into group III (i.e., DINGU, TATB, NTO, FOX-7) have the lower detonation ability compared to the typical (group I) explosives like RDX, HMX. Thus, the testing of the detonability seems to be more efficient in identifying of the group III materials, but during the screening stage when low amount of the sample is available, we are limited to the small- scale testing (DSC, impact and friction sensitivity).

First correlations within safety parameters. [Fig. 6](#_bookmark15) gives a graphical representation of the relationship between the parameters of the ener- getic compounds from [Table 2](#_bookmark16), namely, impact sensitivity - thermal stability (IS-TS), friction sensitivity - thermal stability (FS-TS), and impact sensitivity - friction sensitivity (IS-FS) relationship. As is known, mechanical sensitivity is determined by both mechanical and thermo- kinetic parameters [[72]](#_bookmark94). In particular, the tendency of a decrease in sensitivity with an increase in the critical temperature was discussed [[97,98]](#_bookmark111). However, as can be seen from [Fig. 6](#_bookmark15)a and 6b, there is no strict tendency in IS-TS and FS-TS relationships, and a wide scatter of points along the graph is observed. Obviously, mechanical parameters have an important influence on sensitivity. Additionally, thermal stability determined by thermal analysis corresponds to the critical ignition temperatures at relatively long times ~ 1000 s, whereas in the course of impact tests the reaction commences at much shorter time scale [[8]](#_bookmark43). Some general tendency of parallel changes between the impact and friction sensitivity can be seen in [Fig. 6](#_bookmark15)c. However, there are some materials lying off the general trend. A separate consideration of group II and group III compounds (indicated by color) shows that the outliers cannot be explained by these subsets only.

Sensitivity correlations within certain classes of compounds. We started by checking the correlation of the sensitivity data with previ- ously proposed parameters (descriptors) such as *OB*100, *Q*max (i.e., that are used in Eqs. (1)-(4)). However, among the considered descriptors, a good correlation was found only between the impact and friction sensitivity and the volumetric heat of explosion. The top line in [Fig. 7](#_bookmark27)a shows the results for nitroaromatic explosives: all derivatives of trini-

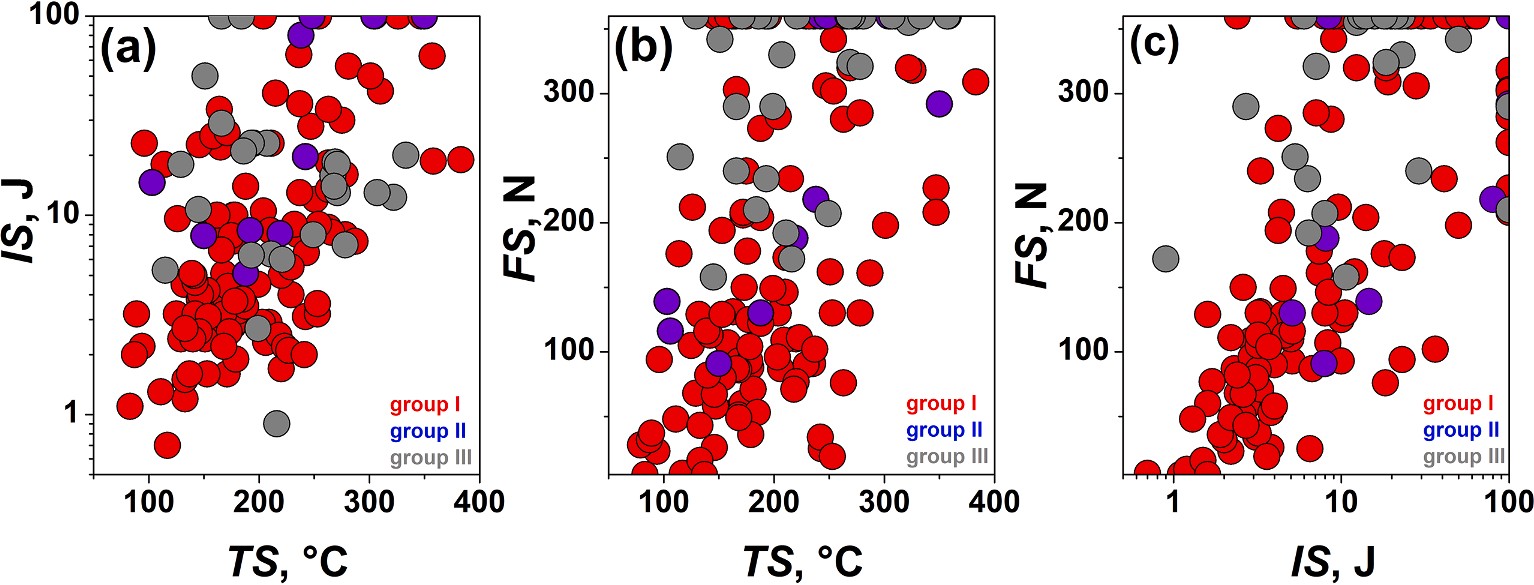
trobenzene fall on the same line in coordinates *IS*-(*ρQ*max). It should be

noted that in this case the correlation is valid for all compounds,

regardless of how the C-NO2 and C–H moieties are located relative to each other, which is different from Kamlet’s observations [[12]](#_bookmark47). The

sensitivity parameters of benzotrifuroxan (BTF, 117) also fall on the line of nitroaromatic compounds, which is in agreement with the studies by Storm [[15]](#_bookmark50) and Wilson [[14]](#_bookmark49).

The introduction of the azido group into nitrobenzenes has been further studied. Compounds **10**, **11** with *para*- and *meta*-position of nitro- and azido-groups have moderate sensitivity, while 1-azido-3,5-



**Fig. 6.** Impact sensitivity - thermal stability (IS-TS, a), friction sensitivity - thermal stability (FS-TS, b), and impact sensitivity - friction sensitivity (IS-FS, c) rela- tionship. Red dots correspond to “normal” energetic materials (group I), blue – to low-energy compounds (group II), gray – to low-sensitive compounds (group III). The graphs are based on the data in [Table 2](#_bookmark16). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

**Table 2**

Impact, friction and thermal sensitivity data for investigated compounds (structural formulas can be found in Supplementary material).

**#** Abbreviation, Chemical name Formula *MP*,

◦C

*TS*,

◦C

*IS*, J *FS*,a [N](#_bookmark17)

1. **ADN**, ammonium dinitramided [[121]](#_bookmark129) H4N4O4 93 150 7.9 ± 0.5 91 ± 6
2. **AP**, ammonium perchlorate H4NO4Cl – 281c 56 ± 12c > 360 (0–20%) c

**3** 2,2,2-Trinitroethanol [[122]](#_bookmark130) C2H3N3O7 72 158 8 ± 3 b

**4 FOX-7**, 2,2-dinitroethene-1,1-diamine [[123]](#_bookmark131) C2H4N4O4 – 207 23 ± 4

107 ± 10b

310 ± 60

**5 BTNEU**, 1,3-bis(2,2,2-trinitroethyl)urea [[124]](#_bookmark132) C5H6N8O13 – 163 3.3 ± 1.1 131 ± 10

**6 TNB**, 1,3,5-Trinitrobenzene C6H3N3O6 122 383 19 ± 6 310 ± 90

**7 PA**, 2,4,6-Trinitrophenol (picric acid) C6H3N3O7 121 247 28 ± 10 310 ± 40

**8** 1-Azido-3,5-dinitrobenzene [[39]](#_bookmark69) C6H3N5O4 83 175 3.3 ± 1.7 240 ± 50

**9 m-DNB**, 1,3-dinitrobenzene C6H4N2O4 90 >350 > 100 292 ± 40

**10** 1-Azido-4-nitrobenzene [[39]](#_bookmark69) C6H4N4O2 70 164 34 ± 9 > 360 (20%)

**11** 1-Azido-3-nitrobenzene [[39]](#_bookmark69) C6H4N4O2 52 165 22 ± 5 > 360 (20%)

**12 TNT**, 2,4,6-trinitrotoluene C7H5N3O6 80 275 30 ± 5 > 360 (0%)

**13 Tetryl**, *N*-Methyl-*N*-(2,4,6-trinitrophenyl)nitramide C7H5N5O8 129 188 14 ± 4 204 ± 20

**14 2,4-DNT**, 2,4-dinitrotoluene C7H6N2O4 69 305 > 100 > 360 (40%)

**15 DNAN**, 2,4-Dinitroanisole C7H6N2O5 87 326 > 100 320 ± 40

1. **NIGU**, Nitroguanidine CH4N4O2 – 166 > 100 300 ± 40
2. **EDNA**, *N*,*N*’-Dinitroethylenediamine C2H6N4O4 177 177 10 ± 3 125 ± 11

**18** 1,1,1,3-Tetranitro-3-azabutane [[125]](#_bookmark133) C3H5N5O8 83 168 5 ± 3 c

**19 RDX**, 1,3,5-Trinitro-1,3,5-triazinane C3H6N6O6 204 204 10 ± 3

93 ± 11 c

130 ± 15

**20 DINGU**, 1,4-Dinitroglycoluril [[126]](#_bookmark134) C4H4N6O6 – 249 8 ± 3 207 ± 22

**21 BC-HMX**, *cis*-2,4,6,8-Tetranitro-1*H*,5*H*-2,4,6,8-tetraazabicyclo[3.3.0]octane [[127]](#_bookmark135) C4H6N8O8 – 235 8.0 ± 0.8 91 ± 25

**22 DNPP**, 1,4-Dinitropiperazine C4H8N4O4 216 251 12 ± 5 c 162 ± 40c

**23 HMX**, 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane C4H8N8O8 280 278 7.6 ± 0.6 e 130 ± 15 e

**24 DATN**, 1,9-Diazido-2,4,6,8-tetranitro-2,4,6,8-tetrazanonane [[128]](#_bookmark136) C H N O

177 177

7.6 ± 1.4 (nano [)](#_bookmark21) 220 ± 20 (nano [)](#_bookmark21)

**25 ZOX**, 1,1,1,3,6,8,8,8-Octanitro-3,6-diazaoctane [[129]](#_bookmark137)

1. **SEX**, Octahydro-1-acetyl-3,5,7-trinitro-1,3,5,7-tetrazocine [[130]](#_bookmark138)
2. **TEX**, 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo[5.5.0.05,9.03,11]-dodecane

5 10 14 8

C6H8N10O16 C6H11N7O7

– 169

219 219

– 267

2.5 ± 0.8 59 ± 10

3.9 ± 1.2 57 ± 8

8.1 ± 0.8 188 ± 30

C6H6N4O8

[[131]](#_bookmark139)

16 ± 2 > 360 (0%)

**28 CL-20**, 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.03,11.05,9]

dodecane [[132]](#_bookmark140)

C6H6N12O12 – 229 4.2 ± 0.5c 80 ± 10c

4.0 ± 0.7 (nanoe[)](#_bookmark21) 110 ± 25 (nanoe[)](#_bookmark21)

1. 4-Methylazide-2,6,8,10,12-pentanitrohexaazaisowurtzitane [[45]](#_bookmark73) C7H8N14O10 – 206 2.3 ± 0.5 87 ± 20
2. 4-(2,2,2-Trinitroethyl)-2,6,8,10,12-pentanitrohexaazaisowurtzitane v C8H8N14O16 – 220 1.7 ± 0.5 77 ± 15
3. 4-(2-Fluoro-2,2-dinitroethyl)-2,6,8,10,12-pentanitrohexaazaisowurtzitane [[47]](#_bookmark75) C8H8FN13O14 – 220 4.9 ± 0.3 110 ± 10

**32** 4-(2-Fluoro-2,2-dinitroethyl)-10-(2,2,2-trinitroethyl)-2,6,8,12-

tetranitrohexaazaisowurtzitane [[47]](#_bookmark75)

C10H10FN15O18 – 209 2.8 ± 0.6 109 ± 10

**33** 4,10-methylazide-2,6,8,12-tetranitrohexaazaisowurtzitane [[45]](#_bookmark73) C8H10N16O8 – 179 2.9 ± 0.2 88 ± 15 **34** 4,10-Bis(2,2,2-trinitroethyl)-2,6,8,10,12-tetranitrohexaazaisowurtzitane [[46]](#_bookmark74) C10H10N16O20 – 216 0.9 ± 0.1 172 ± 30 **35 TNSTAD**, 1,4,5,8-Tetranitroso-1,4,5,8-tetraazadecalin [[133]](#_bookmark141) C6H10N8O4 – 211 6.4 ± 1.2 192 ± 15

1. **ETN**, Erythritol tetranitrate [[134]](#_bookmark142) C4H6N4O12 60 171 1.5 ± 0.3 60 ± 10
2. **PETN**, Pentaerythritol tetranitrate C5H8N4O12 141 181 3.3 ± 0.3 71 ± 10
3. **SMX**, 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethylene)butane [[68]](#_bookmark91) C6H8N6O16 86 168 2.7 ± 0.6 51 ± 10

**39 NC**, Nitrocellulose (11.5% N) (C6H8(NO2)2O5)n – 193 6.3 ± 1.0 f 234 ± 20 f

1. **24-DNI**, 2,4-dinitro-1*H*-imidazole [[135]](#_bookmark143) C3H2N4O4
2. 4,5-dinitro-1*H*-imidazole [[135]](#_bookmark143) C3H2N4O4
3. 4(5)-Nitro-1*H*-imidazole C3H3N3O2

– 269

176 263

304 304

3.5 ± 1.3 (nano [)](#_bookmark22) 340 ± 20 (nano [)](#_bookmark22)

19 ± 3 320 ± 30

9 ± 3 280 ± 40

> 100 > 360 (20%)

**43** 4-Chloro-3,5-dinitro-1*H*-pyrazole [[136]](#_bookmark144) C3HClN4O4 155 287 8 ± 3 160 ± 25

**44 TNP**, 3,4,5-trinitro-1*H*-pyrazole [[137,138]](#_bookmark145) C3HN5O6 186 263 18 ± 3 76 ± 15

**45 34-DNP**, 3,4-dinitro-1*H*-pyrazole [[139]](#_bookmark146) C3H2N4O4 86 263 34 ± 6 > 360 (10%)

**46 35-DNP**, 3,5-dinitro-1*H*-pyrazole [[139]](#_bookmark146) C3H2N4O4 168 310 42 ± 5 > 360 (0%)

**47** 1,3-dinitro-1*H*-pyrazole [[139]](#_bookmark146) C3H2N4O4 66 178 10 ± 3 95 ± 10

**48 4-NP**, 4-nitro-1*H*-pyrazole [[140]](#_bookmark147) C3H3N3O2 161 347 > 100 227 ± 25

**49 3-NP**, 3-nitro-1*H*-pyrazole [[139]](#_bookmark146) C3H3N3O2 174 347 > 100 212 ± 30

**50 1-NP**, 1-nitro-1*H*-pyrazole [[139]](#_bookmark146) C3H3N3O2 91 172 10 ± 6 210 ± 50

**51 5-ADP**, 5-amino-3,4-dinitro-1*H*-pyrazole [[44,141]](#_bookmark72) C3H3N5O4 195 195 23 ± 2 > 360 (40%)

**52** 3,5-Dinitro-1*H*-pyrazol-1-amine [[142]](#_bookmark149) C3H3N5O4 111 278 16 ± 8 160 ± 20

**53** 3-Nitro-1*H*-pyrazol-5-amine C3H4N4O2 193 254 ≈ 100 300 ± 30

**54 ATNP**, Ammonium 3,4,5-trinitropyrazole [[143,144]](#_bookmark150) C3H4N6O6 219 210 8.4 ± 1.4 150 ± 20

**55** 1-(fluorodinitromethyl)-3,5-dinitro-1*H*-pyrazole [[48]](#_bookmark76) C4HFN6O8 91 203 2.9 ± 1.1 100 ± 15

**56** 3-Nitro-1*H*-pyrazole-5-carbonitrile [[145]](#_bookmark151) C4H2N4O2 150 423 > 100 260 ± 25

**57 DNPPy**, 3,6-dinitropyrazolo[4,3-*c*]pyrazole [[146]](#_bookmark152) C4H2N6O4 – 322 12 ± 4 320 ± 25

**58 MTNP**, 1-methyl-3,4,5-trinitro-1*H*-pyrazole [[137,144]](#_bookmark145) C4H3N5O6 90 266 8 ± 3 > 360 (0%)

**59** 4-Methyl-3,5-dinitro-1*H*-pyrazole [[147]](#_bookmark153) C4H4N4O4 203 301 > 50 200 ± 25

**60** 1,2-bis(3,4-dinitro-1*H*-pyrazol-1-yl)diazene [[148]](#_bookmark154) C6H2N10O8 218 218 2.5 ± 1.5 71 ± 9

**61** 1,2-bis(3,5-dinitro-1*H*-pyrazol-1-yl)diazene [[148]](#_bookmark154) C6H2N10O8 – 243 7 ± 3 25 ± 3

**62** 4,4′-Dinitro-2*H*,2′ *H*-3,3′-bipyrazole [[149]](#_bookmark155) C6H4N6O4 303 358 19 ± 8 > 360 (0%)

**63 NTO**, 3-Nitro-1,2,4-triazol-5-one [[150]](#_bookmark156) C2H2N4O3 – 271 13 ± 6c ≈ 360 (40–80%)c

**64 ANTA**, 5-Amino-3-nitro-1*H*-1,2,4-triazole [[151]](#_bookmark157) C2H3N5O2 242 242 20 ± 5 > 360 (0%)

**65 BNT**, 5,5′-dinitro-2*H*,2′ *H*-3,3′-bi-1,2,4-triazole [[152]](#_bookmark158) C4H2N8O4 263 263 14 ± 4 > 360 (0%)

**66** 1,2-Bis(3-nitro-1*H*-1,2,4-triazol-1-yl)diazene [[148]](#_bookmark154) C4H2N10O4 242 242 3.1 ± 0.6 34 ± 11

**67 ANF**, 3-Amino-4-nitrofurazan [[153]](#_bookmark159) C2H2N4O3 122 146 23 ± 9 > 360 (0%)

**68 DNNF**, 3,4-Di(nitramino)furazan [[154]](#_bookmark160) C2H2N6O5 94 94 2.2 ± 0.4 23 ± 3

**#** Abbreviation, Chemical name Formula *MP*,

◦C

*TS*,

◦C

*IS*, J *FS*,a [N](#_bookmark17)

108 151 > 50 > 360 (0%)

|  |  |  |
| --- | --- | --- |
| **103** | 1-(3-nitrophenyl)-1*H*-tetrazole [[174]](#_bookmark178) | C7H5N5O2 |
| **104** | 1-(4-amino-3,5-dinitrophenyl)-1*H*-tetrazole [[175]](#_bookmark179) | C7H5N7O4 |
| **105** | 3-nitro-4-(3-nitrophenyl)-furoxan [[176]](#_bookmark180) | C8H4N4O6 |
| **106** | 4-nitro-3-(3-nitrophenyl)-furoxan [[177]](#_bookmark181) | C8H4N4O6 |
| **107** | 4-(3,5-dinitrophenyl)-3-nitrofuroxan [[58]](#_bookmark84) | C8H3N5O8 |
| **108** | 3,3′-(4-nitro-1,3-phenylene)bis(4-nitrofuroxan) [[178]](#_bookmark182) | C10H3N7O10 |
| **109** | 4,4′-(2-nitro-1,4-phenylene)bis(3-nitrofuroxan) [[178]](#_bookmark182) | C10H3N7O10 |
| **110** | 3-(2,4-dinitrophenyl)-1,2,3,4-oxatriazol-3-ium-5-olate [[39]](#_bookmark69) | C7H3N5O6 |
| **111** | 3-(3,5-dinitrophenyl)-1,2,3,4-oxatriazol-3-ium-5-olate [[39]](#_bookmark69) | C7H3N5O6 |
| **112** | 3-(3-nitrophenyl)-1,2,3,4-oxatriazol-3-ium-5-olate [[39]](#_bookmark69) | C7H4N4O4 |
| **113** | 3-(4-nitrophenyl)-1,2,3,4-oxatriazol-3-ium-5-olate [[39]](#_bookmark69) | C7H4N4O4 |
| **114** | 3-phenyl-1,2,3,4-oxatriazol-3-ium-5-olate [[39]](#_bookmark69) | C7H5N3O2 |

|  |  |  |
| --- | --- | --- |
| **69** | **DAF**, 3,4-Diaminofurazan [[155]](#_bookmark161) | C2H4N4O 180 238 80 ± 8 218 ± 15 |
| **70** | 3-Cyano-4-aminofurazan [[156]](#_bookmark162) | C3H2N4O 83 215 41 ± 13 234 ± 45 |
| **71** | **DNAF**, 3,3′-Dinitro-4,4′-azoxyfurazan [[157,158]](#_bookmark163) | C4N8O7 108 223 2.2 ± 0.6 111 ± 30 |
| **72** | 3-(Nitro-*NNO*-azoxy)-4-{[4-(nitro-*NNO*-azoxy)furazan-3-yl]- azofurazan [[52]](#_bookmark80) | C4N12O8 83 83 1.1 ± 0.2 less than 5 |
| **73** | **DNAAF**, 3,3′-Dinitroamino-4,4′-azoxyfurazan [[67]](#_bookmark90) | C4H2N10O7 – 79 – 28 ± 5 |
| **74** | **DAAzF**, 3,3′-Diamino-4,4′-azofurazan [[153]](#_bookmark159) | C4H4N8O2 – 307 13 ± 7 > 360 (40%) |
| **75** | **DAAF**, 3,3′-Diamino-4,4′-azoxyfurazan [[153]](#_bookmark159) | C4H4N8O3 254 254 9 ± 3 342 ± 20 |
| **76** | Azobis(nitrofurazanyl-*NNO*-azoxy)furazan [[159]](#_bookmark164) | C8N16O10 99 227 2.1 ± 1.2 – |
| **77** | 3-Cyano-4-nitrofuroxan[[160]](#_bookmark165) | C3N4O4 46 132 4.5 ± 1.5 130 ± 20 |
| **78** | 4-Amino-3-cyanofuroxan [[161]](#_bookmark166) | C3H2N4O2 117 96 23 ± 6 c 100 ± 20 |
| **79** | 3-Carbamoyl-4-nitrofuroxan [[162]](#_bookmark167) | C3H2N4O5 114 114 18 ± 7 180 ± 20 |
| **80** | 4-amino-3-(azidocarbonyl)furoxan [[163]](#_bookmark168) | C3H2N6O3 – 133 1.2 ± 0.6 9 ± 2 |
| **81** | 3-Methyl-4-nitrofuroxan | C3H3N3O4 65 189 4 ± 3 270 ± 40 |
| **82** | 4-Methyl-3-nitrofuroxan | C3H3N3O4 40 176 7.4 ± 1.2 180 ± 50 |
| **83** | 3,4-Dicyanofuroxan | C4N4O2 39 204 > 100 280 ± 70 |
| **84** | **DNBF**, 4,4ʹ-Dinitro-3,3ʹ-bifuroxan [[37]](#_bookmark67) | C4N6O8 135 146 3.8 ± 0.5 26 ± 5 |
| **85** | 4-Azido-4′-nitro-3,3′-bifuroxan [[37]](#_bookmark67) | C4N8O6 87 87 2.0 ± 0.7 32 ± 10 |
| **86** | **DDF**, Dinitroazofuroxan [[58,164]](#_bookmark84) | C4N8O8 – 117 0.7 ± 0.2 5.9 ± 0.8 |
| **87** | 3-Methyl-3′-nitro-4,4′-bifuroxan [[165]](#_bookmark169) | C5H3N5O6 104 129 2.4 ± 1.0 70 ± 30 |
| **88** | 3-Nitro-4-cyclopropylfuroxan [[58]](#_bookmark84) | C5H5N3O4 61 211 23 ± 11 170 ± 20 |
| **89** | 3,3′-Dicyano-4,4′-azofuroxan [[161]](#_bookmark166) | C6N8O4 – 168 3.2 ± 0.3 90 ± 30 |
| **90** | 3,3′-Dicarbamoyl-4,4′-azofuroxan [[162]](#_bookmark167) | C6H4N8O6 – 188 3.5 ± 0.6 120 ± 20 |
| **91** | 3,3′-Dimethyl-4,4′-azofuroxan [[166]](#_bookmark170) | C6H6N6O4 – 145 11 ± 5 160 ± 20 |
| **92** | 3,3′-Dimethyl-4,4′-azoxyfuroxan [[167]](#_bookmark171) | C6H6N6O5 172 172 4.5 ± 1.0 210 ± 40 |
| **93** | *N*,*N*’-bis(3-methylfuroxan-4-yl)methylenediamine [[168]](#_bookmark172) | C7H8N8O8 – 125 3.2 ± 0.9 105 ± 25 |
| **94** | **ANPZ**, 2,6-Diamino-3,5-dinitropyrazine [[169]](#_bookmark173) | C4H4N6O4 – 357 63 ± 31 > 360 (10%) |
| **95** | **LLM-105**, 2,6-diamino-3,5-dinitropyrazine-1-oxide [[170]](#_bookmark174) | C4H4N6O5 – 333 20 ± 6 > 360 (40%) |
| **96** | **DAT**, 1*H*-tetrazole-1,5-diamine | CH4N6 188 188 5 ± 3 130 ± 25 |
| **97** | 1′ *H*-1,5′-Bitetrazole [[171]](#_bookmark175) | C2H2N8 184 > 100 210 ± 40 |
| **98** | **ABTOX**, Ammonium 5,5′-bistetrazole-1,1′-diolate [[172]](#_bookmark176) | C2H8N10O2 – 271 18 ± 2 > 360 (10%) |
| **99** | **TKX-50**, Hydroxylammonium 5,5′-bistetrazole-1,1′-diolate [[172]](#_bookmark176) | C2H8N10O4 – 237 36 ± 6 102 ± 10 |
| **100** | **AIBN**, (*E*)-2,2′-(diazene-1,2-diyl)bis(2-methylpropanenitrile) | C8H12N4 103 103 15 ± 4 140 ± 10 |
| **101** | **BPO**, Benzoyl peroxideg | C14H10O4 106 106 – 116 ± 15 |
| **102** | 1-(4-nitrophenyl)-1*H*-tetrazole [[173]](#_bookmark177) | C7H5N5O2 193 23 ± 4 > 360 (0%) |

– 219 6 ± 3

90 162 10 ± 6 c

> 360 (0%)

> 360 (40%)

83 175 8 ± 4 > 360 (20%)

111 153 4.2 ± 0.5 200 ± 50

133 173 2.6 ± 0.5 150 ± 30

– 199 4.5 ± 0.5 150 ± 20

151 151 2.4 ± 0.3 > 360 (0%)

153 229 5.5 ± 0.6 > 360 (10%)

111 237 13 ± 5 > 360 (0%)

167 236 64 ± 12 > 360 (0%)

82 248 > 100 > 360 (0%)

**115 ADNBF**, 7-Amino-4,6-dinitrobenzofuroxanh [[179]](#_bookmark183) C6H3N5O6 268 14 ± 8 > 360 (0%)

**116** 7-Hydroxy-4,6-dinitrobenzofuroxan [[180]](#_bookmark184) C6H2N4O7 – 126 9.6 ± 1.0 210 ± 90

**117 BTF**, Benzotrifuroxan C6N6O6 195 253 2.9 0.5 (orange- pink)g

±

g

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **118**  **119** | 1-(4-Nitro-1*H*-pyrazol-3-yl)-1*H*-tetrazole [[145]](#_bookmark151)  5-(3(5)-Nitro-1*H*-pyrazol-5(3)-yl)tetrazole [[145]](#_bookmark151) | C4H3N7O2 C4H3N7O2 | –  232 | 199  232 | 3.5 ± 1.3 (cream)g 2.7 ± 0.5  9 ± 4 c | 120 ± 20 (cream)g  290 ± 70  > 360 (0%) |
| **120**  **121**  **122**  **123**  **124** | 1-(1-(Fluorodinitromethyl)-4-nitro-1*H*-pyrazol-3-yl)-1*H*-tetrazole [[49]](#_bookmark77)  1-(4-Nitro-1-(trinitromethyl)-1*H*-pyrazol-3-yl)-1*H*-tetrazolei [[49]](#_bookmark77)  **PTX**, 4-amino-3,7,8-trinitropyrazolo-[5,1-*c*][[1,2,4]](#_bookmark38)triazine [[141]](#_bookmark148)  4*H*-[[1,2,3]](#_bookmark38)triazolo[4,5-*c*][[1,2,5]](#_bookmark38)oxadiazole 5-oxidej [[53]](#_bookmark81)  Ammonium 5-oxido-[[1,2,3]](#_bookmark38)triazolo[4,5-*c*][[1,2,5]](#_bookmark38)oxadiazol-4-ide [[53]](#_bookmark81) | C5H2FN9O6  C5H2N10O8 C5H2N8O6 C2HN5O2  C2H4N6O2 | 111  –  –  –  – | 111  133  278  89  185 | 1.3 ± 0.6  1.5 ± 0.4  7 ± 4  3.2 ± 0.3  3.8 ± 0.7 | 48 ± 20c  16 ± 2  290 ± 50  37 ± 13  53 ± 8 |
| **125** | Hydroxylammonium 5-oxido-[[1,2,3]](#_bookmark38)triazolo[4,5-*c*][[1,2,5]](#_bookmark38)oxadiazol-4-ide [[53]](#_bookmark81) | C2H4N6O3 | 123 | 147 | 4.0 ± 1.1 | 58 ± 20 |
| **126** | Hydrazinium 5-oxido-[[1,2,3]](#_bookmark38)triazolo[4,5-*c*][[1,2,5]](#_bookmark38)oxadiazol-4-ide [[53]](#_bookmark81) | C2H5N7O2 | – | 166 | 6.7 ± 1.7 | 87 ± 15 |
| **127**  **128** | Triaminoguanidinium 5-oxido-[[1,2,3]](#_bookmark38)triazolo[4,5-*c*][[1,2,5]](#_bookmark38)oxadiazol-4-ide [[53]](#_bookmark81)  3-(5-(fluorodinitromethyl)-1*H*-1,2,4-triazol-3-yl)-4-nitro-1,2,5-oxadiazole [[50]](#_bookmark78) | C3H9N11O2 C5HFN8O7 | 142  87 | 142  158 | 4.6 ± 1.7  25 ± 6 c | 115 ± 20  > 360 (10%) |
| **129** | (*Z*)-1,2-bis(4-(3-(fluorodinitromethyl)-1*H*-1,2,4-triazol-5-yl)-1,2,5-oxadiazol-3-yl) | C10H2F2N16O10 | 142 | 142 | 3.2 ± 1.7 | 113 ± 20 |
| **130** | 1-(1*H*-1,2,4-triazol-3-yl)-1*H*-tetrazole [[182]](#_bookmark186) | C3H3N7 | – | 186 | 21 ± 4 | > 360 (20%) |
| **131** | 3-(1*H*-1,2,4-triazol-3-yl)-1,2,3,4-oxatriazol-3-ium-5-olate [[183]](#_bookmark187) | C3H2N6O2 | 192 | 192 | 8.4 ± 1.7 | > 360 (0%) |
| **132**  **133** | 7-nitro-3-(nitro-*NNO*-azoxy)-[[1,2,4]](#_bookmark38)triazolo-[5,1-*c*][[1,2,4]](#_bookmark38)triazin-4-amine [[54]](#_bookmark82)  3-(3,4-dinitro-1-(trinitromethyl)-1*H*-pyrazol-5-yl)-4-methylfuroxan [[51]](#_bookmark79) | C4H2N10O5  C7H3N9O11 | –  96 | 154  141 | 3.1 ± 1.3  5.0 ± 1.2 | 80 ± 30  – |
| **134** | 4,4′-dinitro-[3,3′-bi(1,2,5-oxadiazole)] 5-oxide [[38]](#_bookmark68) | C4N6O7 | 96 | 146 | 2.6 ± 0.5 | 67 ± 15 |
| **135** | 4,4′-dinitro-[3,3′-bi(1,2,5-oxadiazole)] 2-oxide [[38]](#_bookmark68) | C4N6O7 | 102 | 140 | 2.4 ± 0.4 | 82 ± 10 |
| **136**  **137** | 4-Nitro-3-(5-amino-1,2,4-oxadiazol-3-yl)furoxan [[184]](#_bookmark188)  **BNAFO**, bis(4-nitro-1,2,5-oxadiazole-2-oxid-3-yl)-azo-1,2,4-oxadiazole [[184]](#_bookmark188) | C4H2N6O5  C8N12O10 | 144  172 | 178  179 | 4.5 ± 2.5  1.9 ± 0.4 | 104 ± 40  36 ± 7 |
| **138**  **139**  **140** | Ammonium 5-(4-azido-2-oxido-1,2,5-oxadiazol-3-yl)tetrazol-1-ide [[55]](#_bookmark83)  Ammonium 4-(1*H*-tetrazol-5-yl)-1,2,5-oxadiazol-3-amine 5-oxide [[185]](#_bookmark189) Guanidinium 5-(4-azido-2-oxido-1,2,5-oxadiazol-3-yl)tetrazol-1-ide [[55]](#_bookmark83) | C3H4N10O2 C3H6N8O2  C4H6N12O2 | –  –  – | 168  171  166 | 2.2 ± 0.5  26 ± 10  29 ± 7 | 49 ± 12  > 360 (0%)  240 ± 60 |

1. ± 20 (orange- pink)

diazene [[50]](#_bookmark78)

**#** Abbreviation, Chemical name Formula *MP*,

◦C

*TS*,

◦C

*IS*, J *FS*,a [N](#_bookmark17)

1. Hydrazinecarboxamidium 5-(4-azido-2-oxido-1,2,5-oxadiazol-3-yl)tetrazol-1-ide [[55]](#_bookmark83) C4H6N12O3 – 139 5.1 ± 0.9 116 ± 20
2. Amino(hydrazinyl)methaniminium 5-(4-azido-2-oxido-1,2,5-oxadiazol-3-yl)tetrazol- 1-ide [[55]](#_bookmark83)

C4H7N13O2 – 129 18 ± 4 > 360 (40%)

1. Triaminoguanidine 5-(4-azido-2-oxido-1,2,5-oxadiazol-3-yl)tetrazol-1-ide [[55]](#_bookmark83) C4H9N15O2 – 133 2.7 ± 0.5 43 ± 9

**144** 3,6,7-Triamino-7*H*-[1,2,4-triazolo[4,3-*b*][[1,2,4]](#_bookmark38)triazol-2-ium 5-(4-azido-2-oxido-

1,2,5-oxadiazol-3-yl)tetrazol-1-ide [[55]](#_bookmark83)

1. Ammonium (*E*)-5,5′-(diazene-1,2-diylbis(2-oxido-1,2,5-oxadiazole-4,3-diyl))bis (tetrazol-1-ide) [[55]](#_bookmark83)
2. Guanidinium (*E*)-5,5′-(diazene-1,2-diylbis(2-oxido-1,2,5-oxadiazole-4,3-diyl))bis

(tetrazol-1-ide) [[55]](#_bookmark83)

C6H7N17O2 – 115 5 ± 3 c 251 ± 50

C6H8N16O4 – 153 1.6 ± 0.5 129 ± 20

C8H12N20O4 – 151 > 50c 342 ± 20

**147 FTDO**, [[1,2,5]](#_bookmark38)oxadiazolo[3,4-*e*][[1,2,3,4]](#_bookmark38)tetrazine 4,6-dioxide [[186]](#_bookmark190) C2N6O3 113 137 1.6 ± 0.2 less than 5

**148 TTTO**, [[1,2,3,4]](#_bookmark38)tetrazino[5,6-*e*]-[[1,2,3,4]](#_bookmark38)tetrazine 1,3,6,8-tetraoxide [[187]](#_bookmark191) C2N8O4 – 158 – –

**149 DNBTT**, 2,9-dinitrobis([[1,2,4]](#_bookmark38)triazolo)[1,5-*d*:5′,1′-*f*][[1,2,3,4]](#_bookmark38)tetrazine [[188]](#_bookmark192) C4N10O4 – 241 2.0 ± 0.4 72 ± 13

**150 TNDPT,** 1,2,9,10-Tetranitrodipyrazolo[1,5-*d*:5′,1′-*f*][[1,2,3,4]](#_bookmark38)tetrazine [[66]](#_bookmark89) C6N10O8 196 253 3.6 ± 0.5 19 ± 4

a When the friction sensitivity is above the maximal limit of the instrument (360 N), in brackets the percent of positive events at 360 N is given.

b See [Fig. 4](#_bookmark13) and its discussion in text.

c An average value is given among several lots of the compound (viz., 12 lots of HMX,10 lots of CL-20, 5 lots of RDX, for other indicated compounds the average of 2 lots is given).

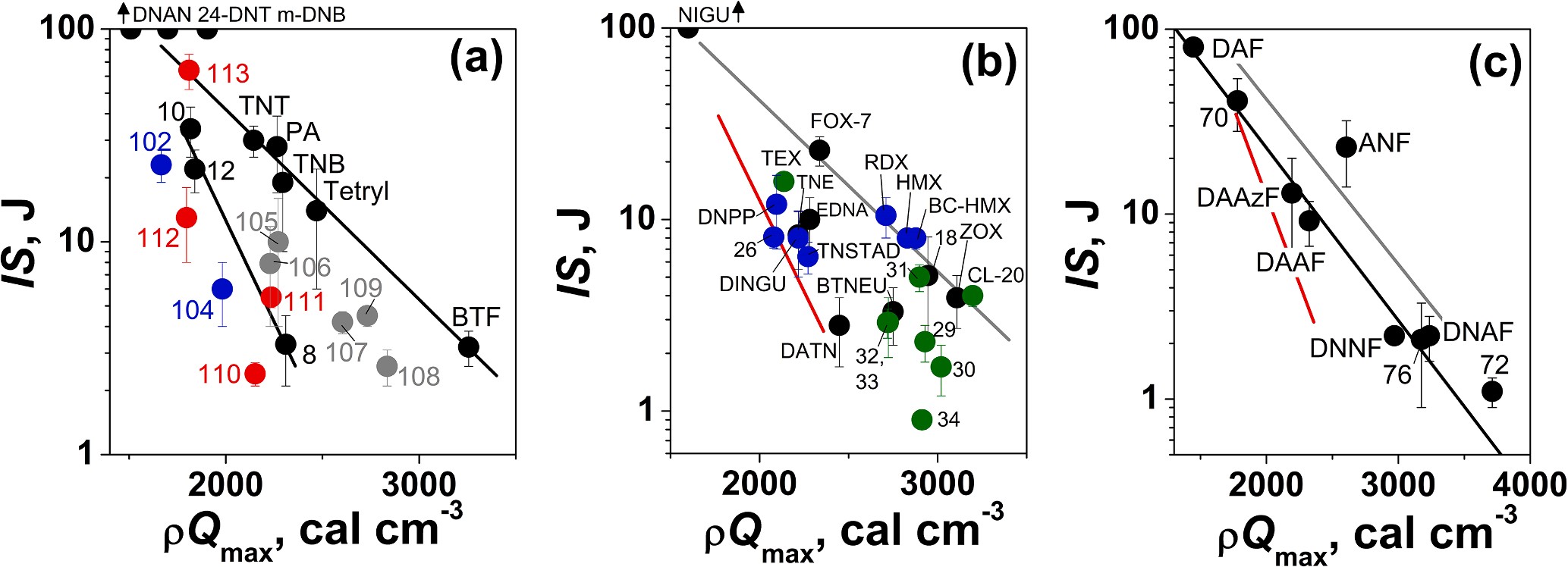
d Commercial granular product.

e Nano-sized laboratory powders produced by spray-drying technique [[80]](#_bookmark99).

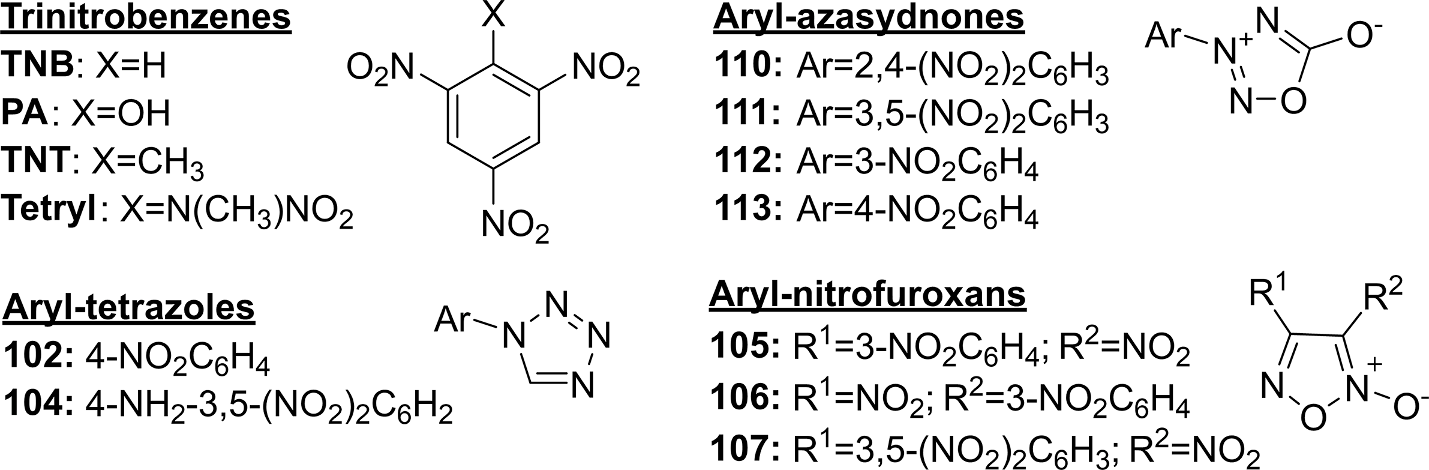
f Nano-sized laboratory powders prepared by supercritical antisolvent processing [[189]](#_bookmark193).

g Commercial product by Acros, having 75% of water. Left in thin layer under room temperature for a few hours till the constant mass.

h Based on recorded 1H and 13C NMR spectra and their comparison with those of known benzofuroxans, the indicated position of amino- group was proved. i The color change takes place upon prolonged exposure to the light. This effect was observed [[190]](#_bookmark194) and possibly relates to different polymorhs of BTF [[191]](#_bookmark195). j The results for potassium salt can be found in original papers.



**Fig. 7.** Correlation of impact sensitivity of nitroaryl- compounds (a), linear, cyclic, cage nitrocompounds (b), and furazans (c) with the computed maximal heat of explosion. Compound numbers and abbreviations correspond to [Table 2](#_bookmark16). Gray and red lines on the plots (b), (c) correspond to the linear approximation of the data for nitroaromatic and nitroazidoaromatic compounds, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



**Scheme 1.** Investigated aryl-substituted compounds.

dinitrobenzene [(8)](#_bookmark36) shows a high impact sensitivity. In total, the azido functionality expectedly sensitizes the molecule, as its linear fit lies lower that line for nitrobenzene derivatives ([Fig. 7](#_bookmark27)a).

In order to estimate the inherent sensitivity of the heterocyclic moieties, they were combined with a nitrobenzene core (see [Scheme 1](#_bookmark28)). It is important to note that the use of the calculated heat of explosion for compounds of this type becomes less accurate, since the enthalpy of their formation is usually also calculated. For arylazasydnones

**110**–**112**, for which experimental enthalpies of formation are available [[39]](#_bookmark69), the position in the graph of [Fig. 7](#_bookmark27)a shows that they are more

sensitive than the corresponding aryl azides **10**–**11**. The only exception

is **113** where the azasydnone ring is placed in *para*-position to the nitrogroup and the compound is not sensitized by the introduction of azasydnone, following the trend of nitrobenzenes. The results for two tetrazole-substituted aryl compounds **102**, **104** are fully consistent with

the arylazasydnones. As for nitrofuroxans **105**–**107**, in the accepted scale, they are located between the azides and nitroaromatic com-

pounds. The heat of explosion for these furoxan derivatives is deter- mined by the calculated enthalpy of formation, and a possible refinement of its value may shift the points on the graph for the corre- sponding compounds. Nevertheless, analyzing the data presented in [Fig. 7](#_bookmark27)a, we can conclude that the sensitivity toward impact of nitro- phenyl compounds increases in the following order of substituents: nitro

group ≥ nitrofuroxan ≥ azido group ≥ azasydnone ≈ tetrazole.

[Fig. 7](#_bookmark27)b shows the *IS*-ρ*Q*max relationships for linear nitro compounds (black circles), cyclic nitramines (blue circles), and cage nitramines

(green circles). It is important to note that some energetic materials from the indicated classes of compounds fall within the linear fit of nitro- benzene derivatives (dots around the gray line in [Fig. 7](#_bookmark27)b). This fact, apparently, was observed by Pepekin, but, as we see from the data for other compounds, the linear correlation of *IS*-*ρQ*max is not global. By considering the location of the specific compound on the plot, one should keep in mind that the selected coordinates reflect not only the sensitivity changes, but the energy content too. A clear example of this relationship is the comparison of the properties of octahydro-1-acetyl-

3,5,7-trinitro-1,3,5,7-tetrazocine (**26**), this compound differs from the benchmark HMX by replacing one of the nitro group with an acetyl one) with HMX. This substitution does not change the impact sensitivity,

which is about 8 J for both compounds, regardless of the fact that the enthalpy of formation decreases (from 81 kJ mol—1 for HMX, to 161

+ —

kJ mol—1 for compound **26**). Correspondingly, the heat of explosion is reduced. Another example is 1,4-dinitropiperazine (DNPP, **22**) with a

relatively low density of 1.64 g cm—3 that reduces further the volumetric heat of explosion.

[Fig. 7](#_bookmark27)c illustrates the *IS*-ρ*Q*max relationships for a set of compounds assembled from a few energetic furazans only. The impact sensitivity in

this series increases almost linearly with an increase in the heat of

explosion from 3,4-diaminofurazan (DAF, **69**) to recently synthesized 3- (nitro-NNO-azoxy)-4-{[4-(nitro-NNO-azoxy)furazan-3-yl]-azofurazan

(**72**) [[52]](#_bookmark80). For comparison, the regression obtained for nitroaromatics (from [Fig. 7](#_bookmark27)a) is also shown in [Fig. 7](#_bookmark27)c by gray and red lines. It can be noted that, at close values of the heats of explosion, furazans are more sensitive than nitroaromatics. Within this series, a deviation was observed for 3-amino-4-nitrofurazan (ANF, **67**), which was less sensitive than expected. Perhaps this is the result of the formation of hydrogen bonds between amino and nitro groups, which provides a stabilizing effect.

Pyrazole is a popular base for the design of energetic compounds. As

a result, a wide variety of nitropyrazoles bearing other explosophore groups (compounds **44**–**62**, **118**–**122**, see [Table 2](#_bookmark16)) was investigated in this study. As can be seen from [Fig. 8](#_bookmark29)a, the points corresponding to two

isomeric dinitropyrazoles (34-DNP, 35-DNP) and trinitropyrazole (TNP) lie above the regression for nitroaromatic explosives (gray line), while the characteristic points of the remaining pyrazoles are localized near the nitroaromatic trend. Based on the location of the points on the [Fig. 8](#_bookmark29)a, it can be concluded that explosophoric fragments located at the nitrogen atom of the ring, for example, fluorodinitromethyl (compound

**55**) or azo (compound **60**) groups, sensitize the sensitivity to the impact of nitropyrazoles.

[Fig. 8](#_bookmark29)b illustrates the friction sensitivity data for nitropyrazoles. For compounds of this series, there is a clear tendency of an increase in sensitivity (decrease in value) to friction with an increase in the volume heat of explosion. The sensitivity increases from 4-nitropyrazole (4-NP,

**48**) to tricyclic 1,2,9,10-tetranitrodipyrazolo[1,5-d:5′,1′-f][[1,2,3,4]](#_bookmark38)-

tetrazine (TNDPT, **150**). A number of deviations from the general trend are also visible here; the dots at the top of the graph represent friction insensitive materials. This group includes the most practically inter- esting compounds, for example, 3,4- (**45**) and 3,5-dinitropyrazoles (**46**),

1-methyl-3,4,5-trinitropyrazole (**58**).

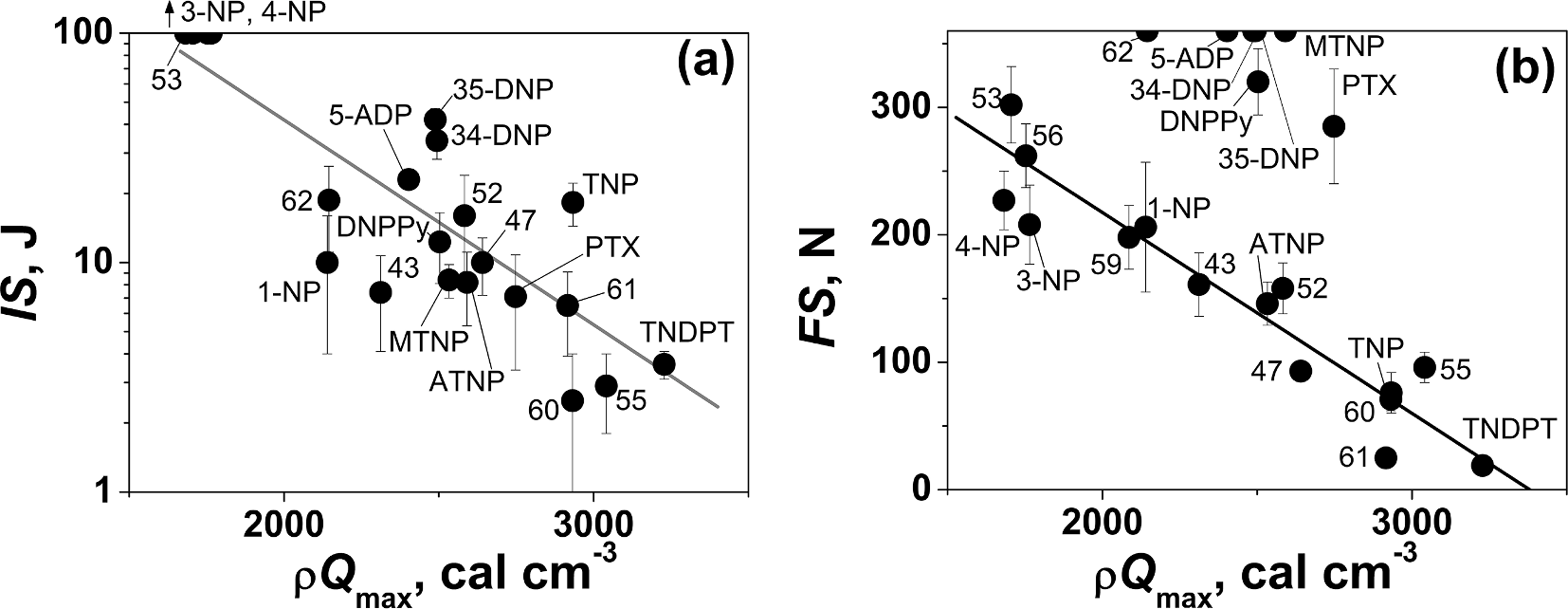
On a general “energy-sensitivity rule”. The relationship between impact and friction sensitivity and volumetric heat of explosion for all

compounds tested in this study is demonstrated in [Fig. 9](#_bookmark30)a and 9b, respectively. As the materials with low energy content (group II) from our list generally have low densities, using of the volumetric heat of explosion effectively shifts the corresponding points to the left side of the graph (blue points, [Fig. 9](#_bookmark30)). Although, as a rule, the sensitivity in- creases with increasing energy content, the observed dependency is not displayed as a single line, as suggested by Pepekin [[22]](#_bookmark56), it looks more

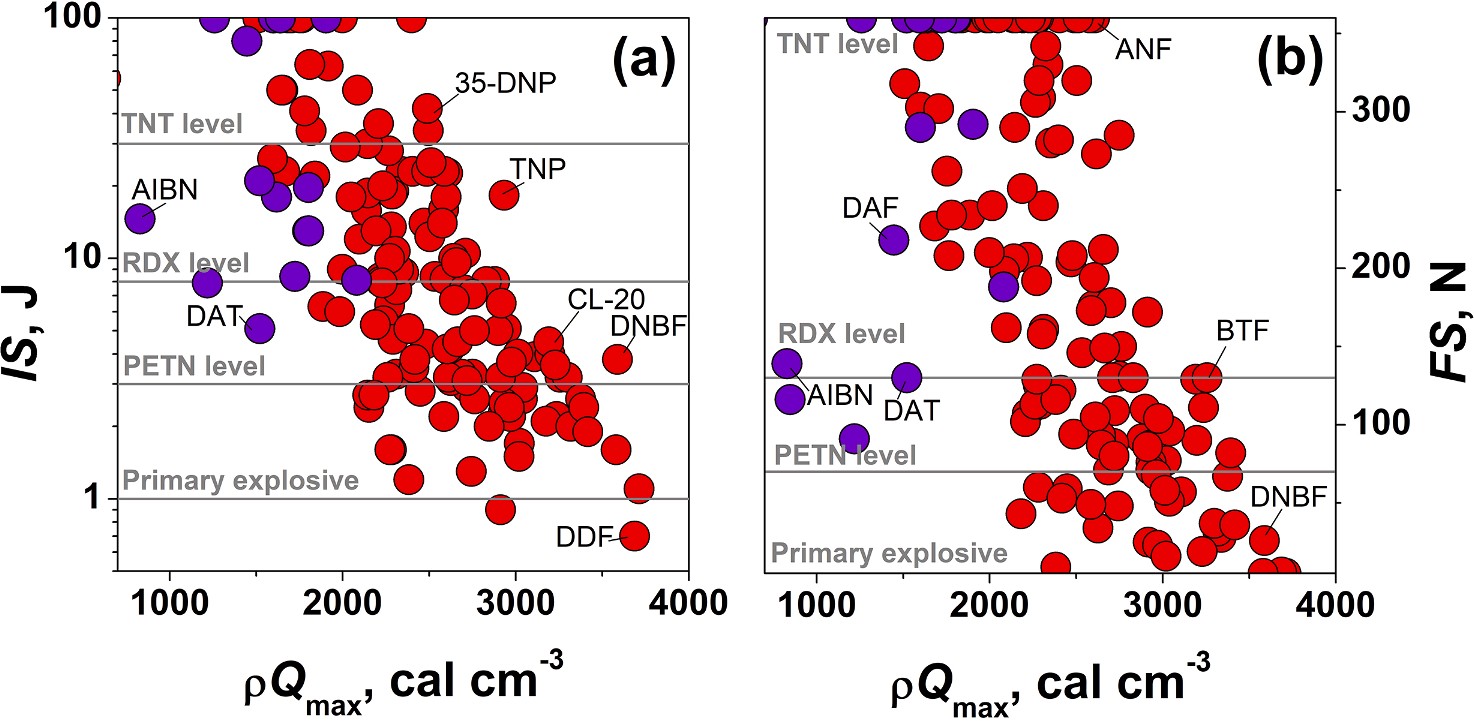
like a “wide path”. Among the possible reasons for this scatter of points

on the graph, the most probable are differences in the mechanical properties of materials and the kinetic factor, which are not considered here. That is, compounds bearing different explosophoric groups obvi- ously have different decomposition mechanisms.

It is interesting to look at the right side of the point cloud in [Fig. 9](#_bookmark30)a



**Fig. 8.** Correlation of impact (a) and friction (b) sensitivity of nitropyrazoles with the computed maximal volumetric heat of explosion. Gray line on plot (a) cor- responds to the linear approximation of similar data for nitroaromatics. Compound numbers and abbreviations correspond to [Table 2](#_bookmark16).



**Fig. 9.** The relationship between impact (a) and friction (b) sensitivity and the volumetric heat of explosion for the compounds of this study. The gray lines represent the sensitivity levels of benchmarks energetic materials. Blue circles denote the compounds of group II. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

and 9b, since the compounds entering this region have a high energy content, but differ significantly in sensitivity. Indicative, for example, is the combination of properties in such high-energy compounds (marked

on the graphs) as 3,5-dinitropyrazole (35-DNP, **46**), 3,4,5-trinitropyra- zole (TNP, **44**), 4,4′-dinitro-3,3′-bifuroxan (DNBF, **84**), hexanitrohex- aazaisowurtzitane (CL-20, **28**). These compounds weave together a high

heat of explosion with acceptable sensitivity, and definitely offer a promise for practical applications.

Based on an analysis of a wide and varied range of energetic mate- rials, we have established a correlation between the mechanical sensi- tivity and the energy content in a compound that requires explanation. Recall that the correlation between the impact sensitivity and heat of explosion was previously noted by Pepekin [[22]](#_bookmark56), Rice [[33]](#_bookmark65), Politzer [[114]](#_bookmark124), and Zeman [[17]](#_bookmark52). Moreover, the correlation suggested by Kamlet (see, Eq. [(1)](#_bookmark4)) between impact sensitivity and the *OB*100 parameter is in fact the same correlation with the heat of explosion: the oxygen content is primarily associated with the formation of detonation products such as CO2 and H2O which increase *Q*max. It is noteworthy that Wilson et al.

[[14]](#_bookmark49) discussing the origin of the dependency of Eq [(1)](#_bookmark4), proposed by Kamlet, associated the oxygen balance with the *propagation* process of detonation, and not with its *initiation*. Support for this idea can be found

Although here we do not discuss the basic considerations and the deri- vation of equations [(5) and (6)](#_bookmark32), both of these semiempirical models suggest a correlation between the mechanical sensitivity and the maximal heat of explosion *Q*max in full agreement with the literature and the results of this study.

In contrast to previous studies, here relationships between energy content and both impact and friction sensitivity were established for energetic compounds of various classes. Taking into account possible errors in the results of determining the impact sensitivity for low- sensitivity and high-melting compounds (see [Fig. 4](#_bookmark13) and its discussion), and striving to work with one sensitivity parameter, we introduce a safety factor, *SF*. *SF* equals the mechanical sensitivity of the compound, normalized so that the TNT value is 100 and the typical value for the primary explosive (1 J or 5 N) is 1. Also, we account other observations from this study: for impact sensitivity we consider the square root of the drop energy *E*50 (because of [Fig. 1](#_bookmark10)a-type dependency), while for friction

sensitivity – friction force *F*50 directly. For compounds from groups I and

II, the SF value is equal to the lowest of the impact or friction sensitiv- ities, for group III, the normalized friction sensitivity data is used only due to likely scatter of the impact sensitivity (see [Fig. 4](#_bookmark13) and its discus-

sion). With this, *SF* is determined as:

in semi-empirical approaches to mechanical sensitivity, as will be shown

( √̅*I*̅*S*̅—1

*FS*—5 )

below.

*SF* = *min* 99 √̅3̅0̅̅—1 +1; 99 360—5 +1 , for groups I, II,

In the past, Belyaev [[115]](#_bookmark125) proposed to divide the probability of the explosion initiation as the product of the probability of the spot exci- tation and the probability of detonation propagation from this spot.

Later, Afanas’ev and Bobolev [[7]](#_bookmark42) theoretically analyzed the mechanical sensitivity under special conditions, expressed as a function of the

minimal diameter (*D*min) of the impactor initiating the explosion:

*SF* = 99 *FS* — 5 + 1, forgroupIII (7)

[Fig. 10](#_bookmark33)a and 10b show the distribution of the safety factor over the mass and volumetric maximal heat of explosion, *Q*max and ρ*Q*max, respectively.

360 — 5

*Dmin* = 2.6

*σ*(*T* )0

*Pcr* — *σ*(*T*0)*dcr*(*T*0, *μ*, *ρ*)

*Tcr* — *MP dcr* (5)

What conclusions can be drawn from the obtained data? [Fig. 10](#_bookmark33)a illustrates the safety factor as a function of the heat of explosion. The limiting compounds are indicated, that are materials delivering the

where σ is the tensile strength, *d*cr – the critical detonation diameter,

*MP*

*T*0 – the initial temperature, *µ* – the average particle size. Equation [(5)](#_bookmark32)

contains two main factors, the first corresponds to the explosion initia- tion, and the second (*d*cr) to the propagation of detonation. The critical diameter, in turn, is inversely proportional to the energy content for secondary explosives [[20]](#_bookmark54), giving rise to the kind of dependency in [Fig. 9](#_bookmark30). For an explosive, Dubovik [[75]](#_bookmark95) proposed a semi-empirical method to estimating the sensitivity parameter (*D*):

*βQmaxρσ*2 *k*

maximal energy at the lowest sensitivity:

Taking into account the difference in density, the list of “limiting”

compounds changes. [Scheme 3](#_bookmark35) shows some compounds from the modified series:

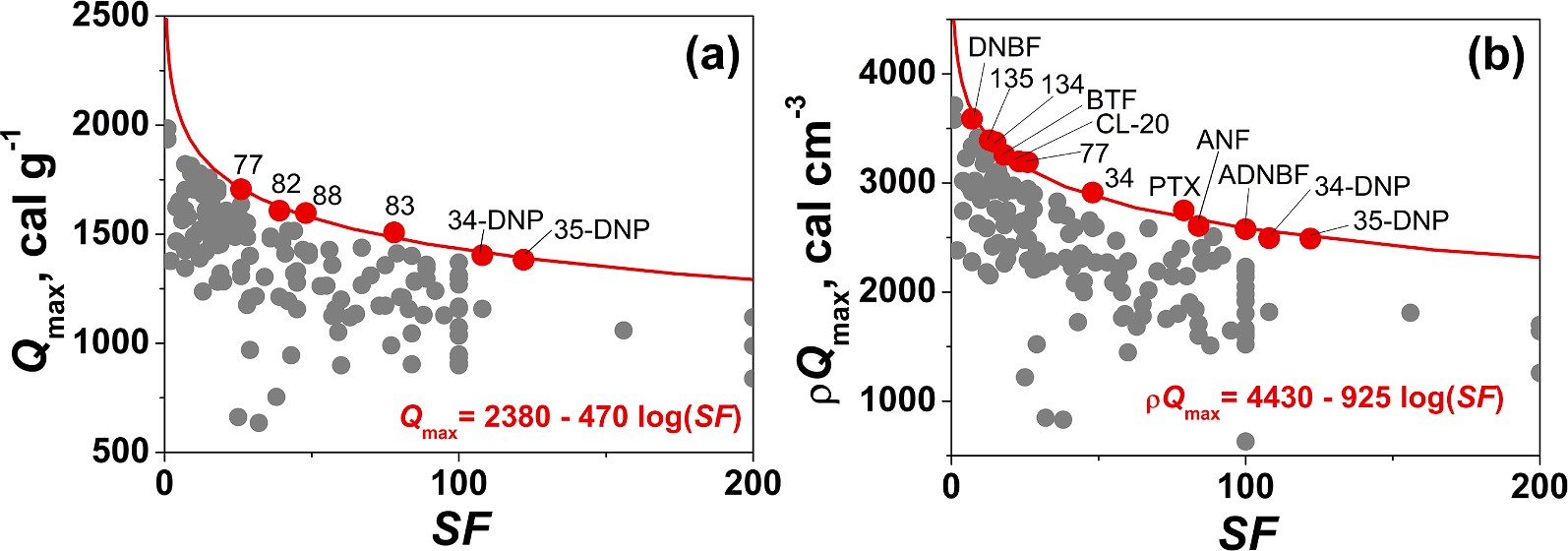
In [Schemes 2 and 3](#_bookmark34), the sensitivity of the compound and *Q*max de- creases systematically from left to right, but the detonation velocity is not in agreement with this trend. This fact was previously noted and analyzed by Politzer and Murray [[114]](#_bookmark124). Here we will try to supplement their observations with an analysis of a wider range of energetic com-

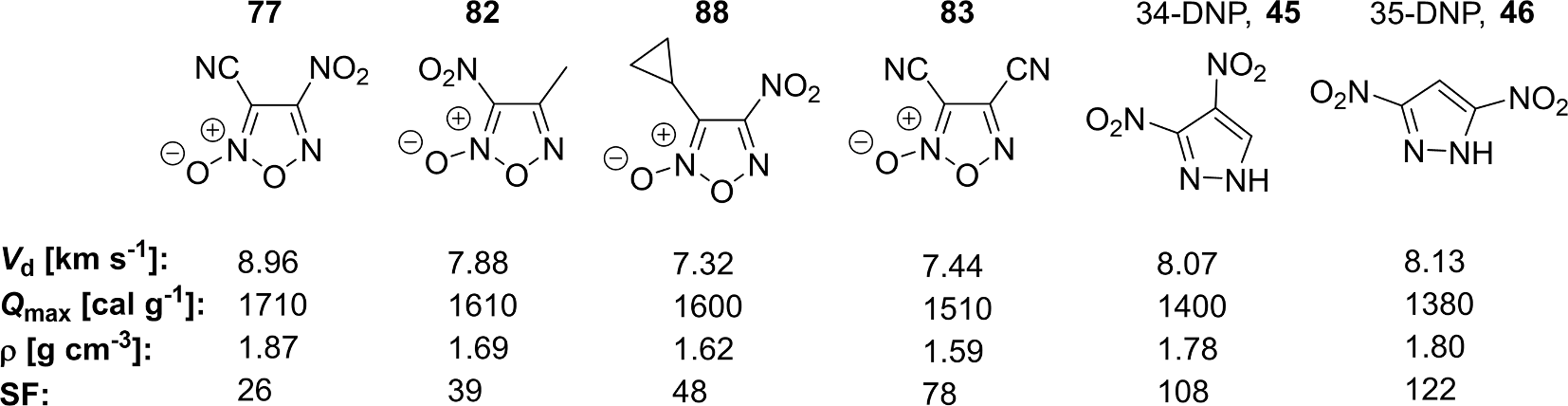
*D* = *Pcr* 4 *dcr* (6)

where *β* is a coefficient, *k* – the constant of the impact machine.

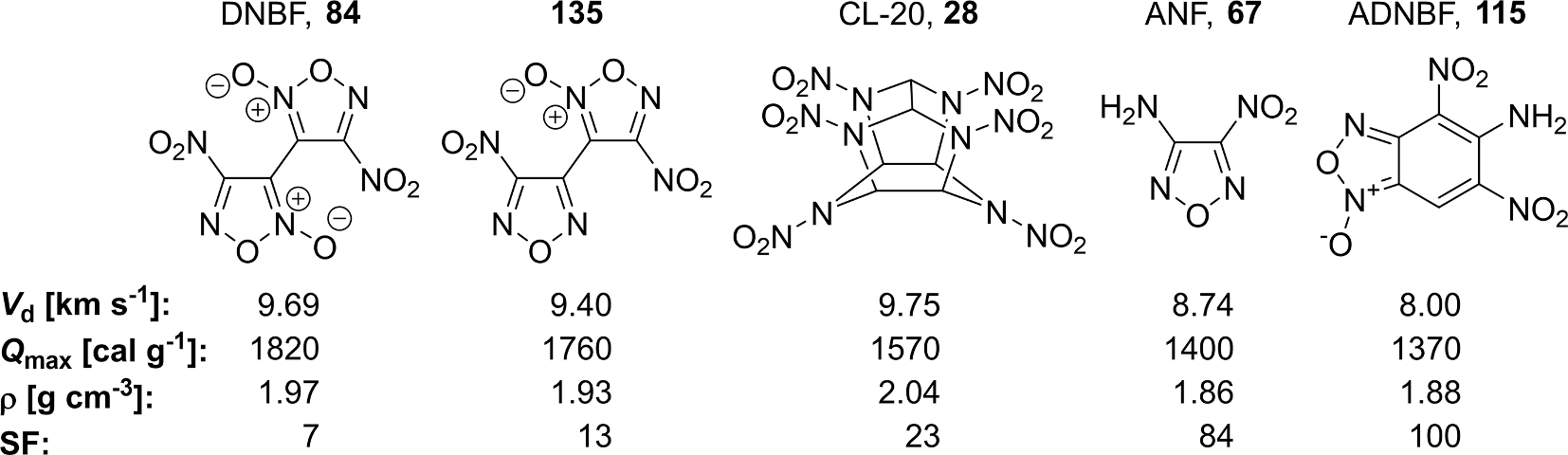
pounds collected in this study. To illustrate how the detonation perfor-

mance is related to the maximal heat of explosion, we will use Pepekin- Lebedev equations [[25]](#_bookmark59). So, the detonation velocity can be described by

**Fig. 10.** The relationship between the safety factor (SF) and (*a*) the maximum heat of explosion and (*b*) the volumetric heat of explosion according to the re- sults of this study. The boundary curve (red) with the currents of compounds lying on it (for discussion, see the text) and the equation describing it (at the bottom of the graph) are presented. For example, typical *SF* values for bench- mark compounds are 100 for TNT, 36 for RDX and HMX, 1 for primary explo- sive. (For interpretation of the refer- ences to color in this figure legend, the reader is referred to the web version of this article.)



**Scheme 2.** The “limiting” compounds on the maximal heat of explosion-sensitivity basis (see [Fig. 10](#_bookmark33)a).



**Scheme 3.** Selected “limiting” compounds on the maximal heat of explosion-sensitivity basis (see [Fig. 10](#_bookmark33)b).

the equation: ([Scheme 3](#_bookmark35)). Both compounds have comparable and high heat of for-

*VD* = 4.2 + 2.0*KEMρ*3/2 (*KPQmax*)1/2 (8)

where the heat realization coefficient is determined as *K*P = 1.014 + 0.122α – 0.0092/(*K*EM∙ρ), α is the oxygen coefficient, and *K*EM is the coefficient taking into account the elemental composition of the mate-

rial and the balance between fuel and oxidizer elements in the molecule. We have previously shown [[37]](#_bookmark67) that equation [(8)](#_bookmark36) offers better accuracy of detonation parameters than several thermodynamic codes and empirical methods, including the well-known Kamlet-Jacobs equations [[26]](#_bookmark60). It should be noted that Pepekin and Lebedev [[25]](#_bookmark59) also proposed equations for calculating other parameters of detonation, for example, the impulse of explosion and detonation pressure, using the same pa- rameters as in Eq. [(8)](#_bookmark36).

As follows from Eq. [(8)](#_bookmark36), density has a stronger effect on the deto- nation performance of a compound in comparison with the heat of ex-

plosion. For example, furoxan **88** has a much higher heat of explosion than benzofuroxan ADNBF, **115** (1600 vs. 1370 cal g—1, see [Schemes 2](#_bookmark34)

[and 3](#_bookmark34)), but its detonation velocity is lower due to the lower density of the crystal (1.62 vs. 1.88 g cm—3, respectively). An even more obvious

advantage of high density is seen when looking at DNBF and CL-20

mation values, but bisfuroxan DNBF has in 16% higher heat of detona-

tion due to more beneficial detonation products. However, only a slight decrease in density, 1.97 g cm—3 for DNBF compared to 2.04 g cm—3 for

CL-20, determined its lower detonation performance. These results can be summarized by the conclusion from Politzer and Murray paper [[114]](#_bookmark124):

“*Q*max needs to be large enough to allow high values of detonation ve- locity and detonation pressure … but not so large as to lead to high sensitivity”. In other words, even if the sensitivity increases with the energy content of the molecule ([Fig. 9](#_bookmark30)), it doesn’t prevent from design of novel compounds with a high detonation performance and appropriate

sensitivity.

We infer a possible application of the dependencies obtained and shown in [Fig. 10](#_bookmark33). In fact, the curves on these plots visually show the state-of-art upper limit of the mechanical sensitivity for energetic ma- terials. The enthalpy of formation required for computation of *Q*max according to Eq. [(3)](#_bookmark3), can be determined experimentally by the calori- metric method, computed theoretically, or obtained by semiempirical method [[116]](#_bookmark126). The state-of-the-art maximum attainable safety factor *SF* is then calculated using one of the equations:

*SF* ≤ 10(2380—*Qmax* )/470 (9)

*SF* ≤ 10(4430—*ρQmax* )/925 (10)

Equation [(10)](#_bookmark37) gives a more conservative estimate of the sensitivity, but the density of the target compound should be known. The obtained safety factor *SF* can be compared directly with its typical values for benchmark energetic materials: 100 for TNT, 36 for nitramines RDX, HMX, 20 for PETN, 1 for primary explosive (e.g., lead azide), or con- verted to the impact and friction sensitivity values (inverse procedure according to Eq. [(7)](#_bookmark31). This procedure may serve to estimate the safety hypothetical structures or to test the adequacy of the experimentally obtained mechanical sensitivity data.

# Summary and outlook

Present paper reports the database of safety parameters determined over the last years at Energetic Materials Laboratory of Semenov Federal Research Center for Chemical Physics. These results were obtained using standard protocols, that are currently accepted within the chemical community. Since the primary goal of this type of analysis is a first assessment of the newly synthesized compounds, it is always a tradeoff between the obtaining a result within an acceptable time on a limited amount of sample and the confidence and broad applicability of this result. The extrapolated onset temperature of the exothermic decom- position peaks seems to be useful for a first rough estimate of the thermal stability of the respective compound. If the analyzed compound vapor- izes in standard conditions of DSC measurement, we propose using the pressure DSC technique [[43,60]](#_bookmark71). A more rigorous thermal stability assessment relevant to storage and operation conditions can be obtained from the kinetic studies and represented by rate constant at an arbitrary temperature [[117,118]](#_bookmark127). Note that when the phase transition occurs before the decomposition peak, the extrapolation of the kinetic data should be done with great care (e.g., [[71,119]](#_bookmark93)).

As for mechanical sensitivity, the present study indicates some problems associated with these tests, especially the determining of response to impact. There are few design types of impact machines in use nowadays (e.g., see [Fig. 5](#_bookmark14) for illustration of the various sample holders). Specifically, the BAM-type device that is common and used in present study, traces its origins to the Kast fall hammer [[120]](#_bookmark128) with chamfered rollers instead of plugs. As it has been discussed in the literature [[8,94]](#_bookmark43), the flow of the sample is hampered in this assembly type, and this phenomenon introduces additional complexity and un- certainty to the deformation process. As we have showed by examples of HMX and CL-20, the powder properties affect the determined impact

sensitivity to some extent. Besides, the using of the loose powder “robs”

some energy for pressing of the sample. The sampling based on a volume instead of mass or pellet height has its pros and cons, exemplified by the results for ultrafine HMX ([Fig. 3](#_bookmark12)). Overall, a more rigorous procedure may involve for each particular sample: (i) a search for the critical height of thin pressed pellets where the maximum of drop energy is absorbed by the sample, [(2)](#_bookmark6) a measurement of this actual energy versus the nominal energy of the falling drop, [(3)](#_bookmark3) two series of tests with an unconfined sample and with guide ring (preferentially with flat, not- chamfered rollers [[8,94]](#_bookmark43)). Obviously, such a detailed study is not possible during the high-throughput screening stage with the limited amount of sample, but some refinements of the standard procedure can be done as it will be discussed in the future study.

The comparison of the impact sensitivity data obtained in the present study with the results by the most rigorous method (*P*cr technique) shows the unexpectedly good agreement. This analysis of data for 18 energetic materials serves as a verification of the method used for obtaining of impact and sensitivity data in present work. All sensitivity data have been reported for 150 CHNOFCl compounds. Analysis of the mechanical sensitivity data in the frame of the sensitivity-energy content correlations shows several interesting trends. Generally, the sensitivity- energy data manifests itself not as a straight line as predicted by Pepe- kin, but more like as a “strip”. Obvious reasons for the scatter in data are

the wide difference in mechanical properties and decomposition mechanisms. However, even such a general correlation gives important implications for the design of energetic materials. The larger heat of explosion is generally accompanied by the higher mechanical sensi- tivity. However, the detonation performance is more affected by the density of the compound rather than its maximal heat of explosion. As an example, hexanitrohexaazaisowurtzitane CL-20 outperforms com- pounds with much higher *Q*max values (DNBF, **135**, [Scheme 3](#_bookmark35)). There- fore, the previously established correlation between the heat of explosion and the mechanical sensitivity does not preclude the existence of a material with high detonation performance and not high sensitivity. As a practical tip for the design of novel energetic materials, two correlations of the general mechanical sensitivity expressed as a safety factor *SF* with the maximal heat of explosion by mass or volume are proposed. This calculation, obviously, will not replace the experimental assessment of mechanical sensitivity, but can support the experimental result, if the relative ranking of material is the same, or guide the syn-

thetic efforts if hypothetical structures are considered [[181]](#_bookmark185)

# Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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# Appendix A. Supplementary data

Supplementary data to this article can be found online at [https://doi.](https://doi.org/10.1016/j.cej.2021.129804) [org/10.1016/j.cej.2021.129804](https://doi.org/10.1016/j.cej.2021.129804).

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