

**Study of Detonation Parameters of  
Polynitroadamantanes, Potential New Explosives.  
I. Molecular Mass/Density and Oxygen  
Content/Sensitivity Relationships.\***

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Molecular mass/density and oxygen content/sensitivity relationships of polynitroadamantanes and their aliphatic counterparts, important for their explosive properties, were studied. Densities, sensitivities and detonation properties of polynitroadamantanes obtained/calculated are the same as those of standard high explosives. Some of them might have better characteristics than TNT, and similar ones to pentrit and hexogen, respectively. Their aliphatic counterparts might be exceptionally sensitive and could have a high energy content, which excludes them from possible use as high explosives.

## INTRODUCTION

There is currently considerable interest in new high energy oxidizers for solid propellants and new high explosives. Polynitropolycyclic cage systems have been at the forefront in the search for such compounds over the past decade.<sup>1</sup> Their good explosive characteristics are a direct result of high crystal densities, particularly in combination with high strain energies built

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into the cage molecule.<sup>2</sup> Polynitroadamantanes, as a class of nitrated cage compounds, are recognized as very promising explosives and/or propellants with a high degree of thermal stability.<sup>3</sup>

Compounds used in highly energetic compositions must satisfy a number of well-known requirements. In addition to the high value of energy content and high crystal density, they should have good stability and low sensitivity to external stimuli.<sup>4</sup> In order to predict such compounds, reliable methods of theoretical evaluation of explosive performance parameters are of principal importance. Such an approach will help avoid possible long and expensive synthetic procedures, thus reducing the cost of synthesis. Also, knowledge of explosive parameters of such compounds will contribute to their efficient and safe application as components of energetic materials.

In our recent work,<sup>5</sup> heats of formation, crystal densities, detonation velocities and pressures for various polynitroadamantanes were calculated, using simple and fast, but quite reliable procedures. Aim of this work is to study the molecular mass/density relationship important for explosive performance parameters of aliphatic polynitro compounds and their adamantane counterparts (Scheme 1). Also, in this work we have studied the relationship between sensitivity and oxygen balance, which could help us in future synthesis decisions as well as in handling these substances.

## THEORY

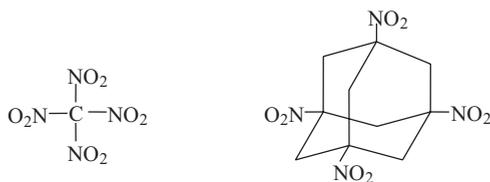
Rigid and compact adamantane nucleus has four bridgehead bonds directed towards the corners of the tetrahedron.<sup>6</sup> By replacing the tetrahedral carbon atom in tetranitromethane (N-1) with adamantane, the known tetranitroadamantane (DS-1) is formed (Formula 1). Similarly, replacing the quaternary carbon in hypothetical tetranitrate (N-2) one comes out with the adamantane counterpart, the known tetranitrate (DS-2).

By applying the same procedure, *i.e.* by replacing the quaternary carbon in neopentyl compounds bearing C-NO<sub>2</sub>, C-ONO<sub>2</sub>,\* and C-NHNO<sub>2</sub> groups, resp. (N-series, Scheme 1) with adamantane, polynitroadamantane counterparts were obtained (DS-series, Scheme 1).

Introducing nitro groups into both frameworks will increase densities and energy contents of the compounds formed. Aliphatic polynitro compounds would have higher densities and higher energies, but would be very reactive and much too sensitive. The rigid symmetric adamantane framework could allow more nitro groups to be introduced. This could possibly give explosives with good performance characteristics and with sensitivities

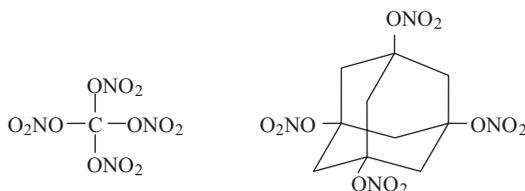
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\* With four ONO<sub>2</sub> groups, known pentrit or PETN (N-6, Scheme 1)



N-1

DS-1



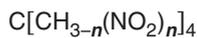
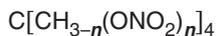
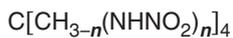
N-2

DS-2

Formula 1

## Aliphatic polynitrocompounds

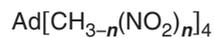
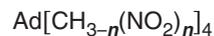
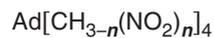
## N-series

 $n=1$ , N-3 $n=2$ , N-4 $n=3$ , N-5 $n=1$ , N-6 $n=2$ , N-6a $n=3$ , N-6b $n=1$ , N-7 $n=2$ , N-7a $n=3$ , N-7b

## Adamantane polynitrocompounds

## DS-series

Ad = adamantane-1,3,5,7-tetrayl

 $n=1$ , DS-3 $n=2$ , DS-4 $n=3$ , DS-5 $n=1$ , DS-6 $n=2$ , DS-6a $n=3$ , DS-6b $n=1$ , DS-7 $n=2$ , DS-7a $n=3$ , DS-7b

Scheme 1. Aliphatic polynitrocompounds (N-series) and Adamantane polynitrocompounds (DS-series)

acceptable for synthetic and production purposes. In addition to the fact that  $\text{NO}_2$  groups contribute to increasing the molecular density, they also contribute to the oxygen balance. Kamlet and Adolph<sup>7</sup> introduced the quantity  $OB_{100}$  as a measure of oxygen balance.\* They established a meaningful relationship between sensitivities of organic explosives and  $OB_{100}$  values for a wide variety of organic compounds.

Density is one of the most significant physical properties of an energetic material.<sup>8</sup> Important performance parameters, such as detonation pressure and velocity increase with density. For example, the detonation pressure of an explosive increases as the square of its density.<sup>9</sup>

## RESULTS AND DISCUSSION

We have calculated detonation parameters for the studied compounds (Scheme 1) using our own computer program EXPLO5.<sup>10,11</sup> The program is based on the steady state model of detonation, BKW equation of state for gaseous products, and the Cowan-Fickett equation of state for solid carbon. EXPLO5 has been tested on a number of known explosives and good agreement between calculated and experimental values has been obtained: the correlation coefficient for detonation velocity calculation was 0.9976 and for detonation pressure was 0.9844.<sup>11</sup>

Input data were: atomic structure (molecular formula) of the compound, its density and enthalpy of formation.

Densities were calculated using Cady's method.<sup>12</sup> This method is theoretical in nature – based on calculation of hard-sphere volume from bond lengths and van der Waals radii – but includes an empirical packing coefficient. Cady's procedure enables one to calculate crystal densities of organic compounds with the standard error of about  $0.07 \text{ g cm}^{-3}$ . This level of accuracy makes Cady's method useful for density calculations of potential energetic compounds.

Enthalpies of formation were calculated using the method developed by Kizin and Lebedev.<sup>13</sup> Their method belongs to the group additivity methods, but it takes into account interactions between individual groups, which makes it very useful for the enthalpy of formation calculation of polynitrocompounds. This method enables one to calculate enthalpies of formation of compounds in their solid states, with a standard error of  $2.5 \text{ kJ mol}^{-1}$ . This level of accuracy makes this method quite reliable, since the detonation ve-

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\*  $OB_{100}$  is the number of equivalents of oxidant *per* hundred grams of explosive above the amount required to burn all hydrogen to water and all carbon to carbon monoxide.<sup>7</sup>

locity is a very weak function of the enthalpy of formation of an explosive.<sup>5,11</sup>

Impact sensitivities were calculated according to the Kamlet and Adolph method (*vide infra*).<sup>7</sup>

Results of calculations of crystal densities, enthalpies of formation, detonation velocities and pressures, are summarized in Table I.

TABLE I  
Detonation properties of Polynitrocompounds – our results

Comp- ound	Brutto formula	Mol. mass g mol <sup>-1</sup>	$\rho_0$ g cm <sup>-3</sup>	$\Delta h_f^0$ J g <sup>-1</sup>	$OB_{100}$ %	$D$ m s <sup>-1</sup>	$p$ GPa	$q$ J g <sup>-1</sup>	$OB_{100}$	$h_{50}$ cm
DS-1	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>8</sub>	316.22	1.583	-1084	-91.1	6990	19.0	-4800	-5.06	2325
DS-2	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>12</sub>	380.22	1.659	-1506	-58.9	7685	23.9	-5470	-2.10	253
DS-3	C <sub>14</sub> H <sub>20</sub> N <sub>4</sub> O <sub>8</sub>	372.32	1.434	-1430	-128.9	6618	15.0	-4014	-8.59	30216
DS-4	C <sub>14</sub> H <sub>16</sub> N <sub>8</sub> O <sub>16</sub>	552.33	1.681	-1138	-57.9	7751	24.4	-5277	-2.17	266
DS-5	C <sub>14</sub> H <sub>12</sub> N <sub>12</sub> O <sub>24</sub>	732.33	1.827	-474	-21.8	8372	32.1	-6397	1.09	24.0
DS-6	C <sub>14</sub> H <sub>20</sub> N <sub>4</sub> O <sub>12</sub>	436.33	1.508	-1528	-95.3	6855	17.7	-4974	-5.50	3091
DS-6a	C <sub>14</sub> H <sub>16</sub> N <sub>8</sub> O <sub>24</sub>	680.32	1.672	-1418	-28.2	7824	25.9	-6094	0.59	34.8
DS-6b	C <sub>14</sub> H <sub>12</sub> N <sub>12</sub> O <sub>36</sub>	924.32	1.792	-1302	3.5	8127	30.1	-6290	3.46	4.2
DS-7	C <sub>14</sub> H <sub>24</sub> N <sub>8</sub> O <sub>8</sub>	432.40	1.458	-821	-118.4	7142	17.7	-4032	-8.33	24784
DS-7a	C <sub>14</sub> H <sub>24</sub> N <sub>16</sub> O <sub>16</sub>	672.47	1.625	109	-57.1	7960	25.3	-5666	-2.97	480
DS-7b	C <sub>14</sub> H <sub>24</sub> N <sub>24</sub> O <sub>24</sub>	912.54	1.745	373	-28.1	8511	31.3	-6215	-0.44	74.2
N-3	C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>8</sub>	252.12	1.607	-1127	-38.1	7803	24.5	-5887	-0.79	96.3
N-4	C <sub>5</sub> H <sub>4</sub> N <sub>8</sub> O <sub>16</sub>	432.15	1.906	-162	14.8	8417	33.3	-5576	4.16	2.5
N-5	C <sub>5</sub> N <sub>12</sub> O <sub>24</sub>	612.15	2.071	1183	36.6	10431 <sup>a</sup>	52.2 <sup>a</sup>	<sup>c</sup>	6.21	0.6
N-6	C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>12</sub> (PETN)	316.40	1.706	-1649	-10.1	8172	29.1	-6444	1.89	13.3
N-6a	C <sub>5</sub> H <sub>4</sub> N <sub>8</sub> O <sub>24</sub>	560.14	1.978	-1599	34.27	7972	27.8	-2855	6.07	0.6
N-6b	C <sub>5</sub> N <sub>12</sub> O <sub>36</sub>	804.13	2.144	-1342	51.73	8182 <sup>a</sup>	32.3 <sup>a</sup>	<sup>c</sup>	7.71	0.2
N-7	C <sub>5</sub> H <sub>12</sub> N <sub>8</sub> O <sub>8</sub>	312.26	1.612	-673	-40.9	8047	25.5	-5321	-1.92	221.0
N-7a	C <sub>5</sub> H <sub>12</sub> N <sub>16</sub> O <sub>16</sub>	552.29	1.833	-320	0	8888	35.5	-5958	1.81	14.1
N-7b	C <sub>5</sub> H <sub>12</sub> N <sub>24</sub> O <sub>24</sub>	792.36	1.941	47	16.15	8842	35.3	-4447	3.28	4.8
RDX	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	222.13	1.806 <sup>b</sup>	318 <sup>b</sup>	-21.6	8854	34.8	-6323	0	53.7
HMX	C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	296.17	1.903 <sup>b</sup>	253 <sup>b</sup>	-21.6	9272	39.4	-6527	0	53.7
TNT	C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	227.13	1.654 <sup>b</sup>	-262 <sup>b</sup>	-73.9	7073	20.9	-5446	-3.08	135
PETN	C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>12</sub>	316.14	1.770 <sup>b</sup>	-1680 <sup>b</sup>	-10.1	8422	31.6	-6749	1.89	13.3
DATB	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	243.13	1.788 <sup>b</sup>	-485 <sup>b</sup>	-55.9	8008	27.2	-4900	-2.06	244

a – calculated according to Kamlet and Jacobs method<sup>9</sup>

b – experimental data (according to Kohler and Meyer)<sup>14</sup>

c – uncalculable by EXPLO5

### Molecular Mass/Density Relationship

Calculated density values were correlated with molecular mass values for C-NO<sub>2</sub>, C-ONO<sub>2</sub> and C-NHNO<sub>2</sub> compounds, Figure 1.

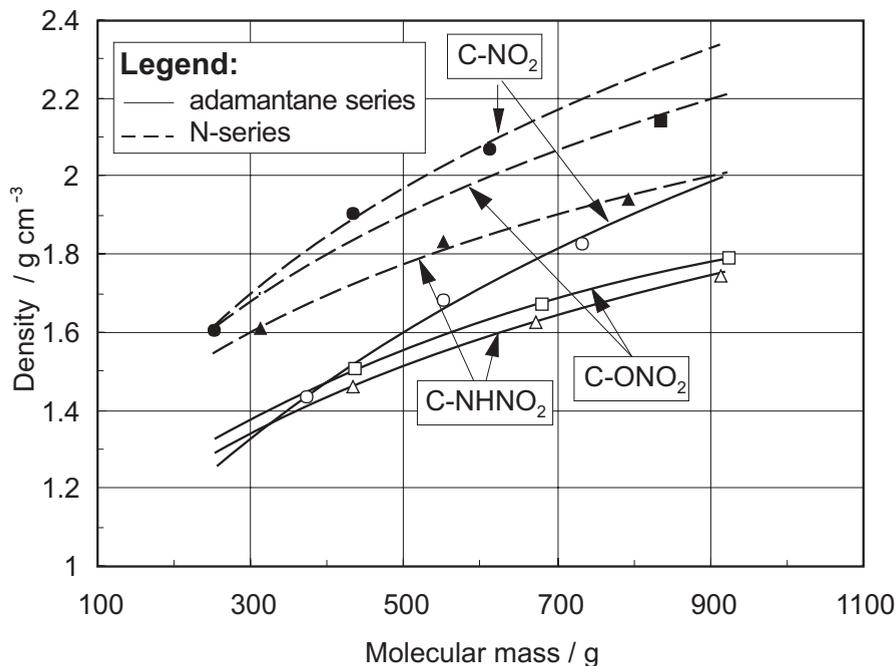


Figure 1. Molecular mass–density relationship.

It is evident that density increases with molecular mass, which in turn increases with increasing number of nitro groups introduced onto the basic molecule framework. According to Sollott *et al.*,<sup>2</sup> it is expected that such an increase would be linear. However, in both series of our compounds this increase is nonlinear.

Such increase of density *vs.* mass is the result of the structure of a particular group, complex steric hindrance, nonbonding interactions, electrostatic effects, *etc.* Using Cady's approach, such behaviour may be explained by the fact that the volume of the group depends both on the attached atom(s) and valence bond(s) within the group. Since the volume of the group is calculated assuming a standard attached atom, volume corrections for the length of attachment bond and for the kind of attached atom must be applied. For example, according to Cady's table, volume correction for C–N bond is equal to 0.54 cm<sup>3</sup> mol<sup>-1</sup>, for C–OR 0.76 cm<sup>3</sup> mol<sup>-1</sup>, while there is no correction for C–C bond (it is equal to zero).

In addition, successive substitution by C-NO<sub>2</sub> groups causes a more rapid increase in densities than in C-ONO<sub>2</sub> and C-NHNO<sub>2</sub> series. Such behaviour results from the fact that C-NO<sub>2</sub> increment has smaller mass and volume than C-ONO<sub>2</sub> and C-NHNO<sub>2</sub>. With more substitution, these differences become greater, and the consequence is an even greater difference in molecular densities, being the greatest for totally substituted carbons.

Compounds from N-series ( N-5, N-6b, and N-7b, resp.) have higher density values than their adamantane counterparts (DS-5, DS-6b, and DS-7b, resp.) (Scheme 1). This was expected, since in N-compounds substituents occupy a closer space than in adamantane derivatives.

The highest density values (Table I) were obtained for adamantane derivatives DS-5 (1.827 g cm<sup>-3</sup>), DS-6b (1.792 g cm<sup>-3</sup>) and DS-7b (1.745 g cm<sup>-3</sup>), while densities for N-series exceed 2 g cm<sup>-3</sup> (2.144 g cm<sup>-3</sup> for N-6b, and 2.071 g cm<sup>-3</sup> for N-5).

### *Oxygen Content/Impact Sensitivity Relationship*

According to Kamlet and Adolph, the impact sensitivity of an explosive is a function of the rates of thermal decomposition processes taking place in temperature regimes generated by the impact of the hammer.<sup>7</sup> These authors have found that a good correlation between the impact sensitivity and the *OB*<sub>100</sub> quantity exists for a number of explosives having a similar decomposition mechanism, *i.e.* similar structure.

Compounds that are the subject of our work lack α-CH linkage, and the following equation<sup>7</sup> was used for calculation of logarithmic 50% impact heights (*h*<sub>50%</sub>):

$$\log h_{50\%} = 173 - 0.32 \cdot OB_{100} \quad (r = 0.96)$$

Using this equation, the correlation coefficient was found to be 0.96, which makes this method reasonably successful in predicting the impact behaviour of new, yet-to-be synthesized explosives.

Calculated logarithmic 50% impact heights of all compounds are plotted against the *OB*<sub>100</sub> values, Figure 2.

One can see that there is a general increase in impact heights, *i.e.* a decrease of impact sensitivity, with decreasing *OB*<sub>100</sub>.

Taking into account that impact heights for the majority of standard high explosives lie between 10–12 cm (*e.g.* for pentrite) and about 300 cm (*e.g.* for 1,3,5-triamino-2,4,6-trinitrobenzene), and that impact heights for primary explosives are below 10 cm (*e.g.* 2–4 cm for lead azide),<sup>7,15</sup> one may classify these compounds into three groups:

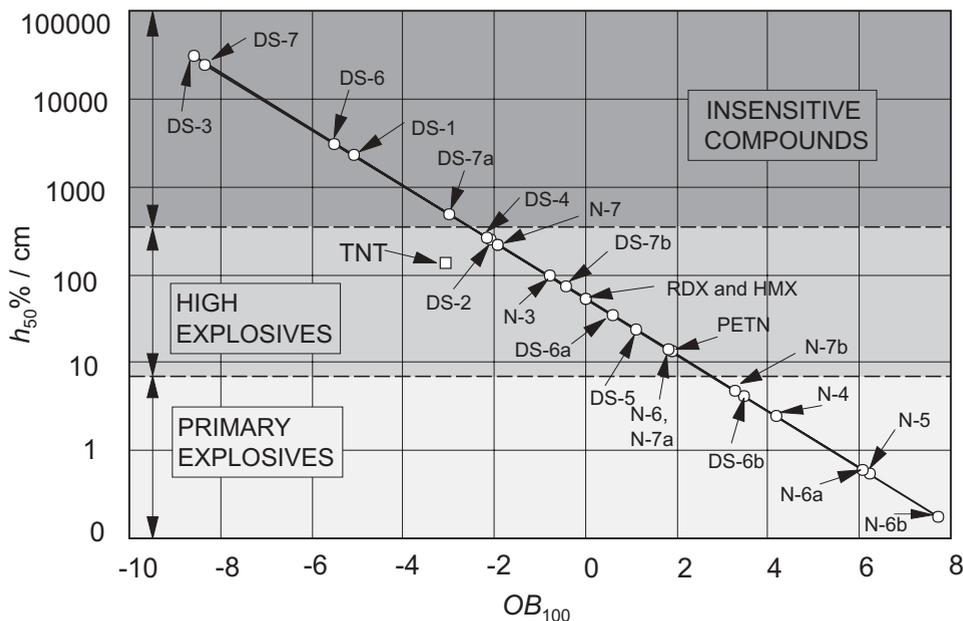


Figure 2. Impact sensitivity- $OB_{100}$  relationship.

a) Compounds having  $h_{50\%}$  value below 10 cm (such as some compounds that belong to N-series: N-6b, N-5, N-6a, N-4, N-7b, and only DS-6b from adamantane series),

b) Compounds having impact heights between 10 and 300 cm (such as N-6, N-7a, N-3, and N-7 from N-series, and DS-5, DS-6a, DS-7b, DS-2, and DS-4 from adamantane series)

c) Compounds having impact heights above 300 cm (such as compounds DS-7a, DS-1, DS-6, DS-7 and DS-3 from adamantane series)

Compounds that belong to group (a) may be considered very sensitive – their sensitivities are in the range of primary explosives, while compounds that belong to group (b) have sensitivities in the range of standard high explosives: TNT – 160 cm, RDX – 22–24 cm, HMX – 24–26 cm, Tetryl – 32–35 cm, *etc.*

Compounds with logarithmic  $h_{50\%}$  impact heights above 300 cm, may be considered insensitive. This group includes 1,3,5,7-tetra(nitromethyl)adamantane DS-3 and 1,3,5,7-tetra(nitraminomethyl)adamantane DS-7, with predicted impact heights of 302 and 248 m, respectively. Known 1,3,5,7-tetranitroadamantane (DS-1) and tetranitrate DS-6 with predicted impact heights of 23 and 31 m, respectively, are also insensitive on impact. Pre-

dicted impact heights of these four compounds are at least 15 times greater than the impact height of TNT.

It should be noted that Kamlet and Adolph<sup>7</sup> have established the  $h_{50}\%$ - $OB_{100}$  correlation using  $OB_{100}$  values ranging between  $-3.5$  and  $2$ . This means that  $h_{50}\%$  values calculated for  $OB_{100}$  values well outside this range may be unrealistic. Anyway, calculated  $h_{50}\%$  values may be taken as a good indicator of sensitivity level, and may be used for the prediction of that level of new, yet-to-be synthesized explosives.

It is shown that a molecule starts becoming an explosive when the degree of nitro substitutions is sufficiently high, depending on molecular structure (*e.g.* in nitroaromatic compounds this degree is 3 per ring).<sup>15</sup> This means that there is a point of nitro substitution above which molecules are explosives. Since the predicted impact heights of some compounds from group (c) are far above 10000 cm, perhaps such compounds could not be considered explosives.

An increase of nitro substitution causes an increase of impact sensitivity, *i.e.* a decrease of impact height (Figure 3).

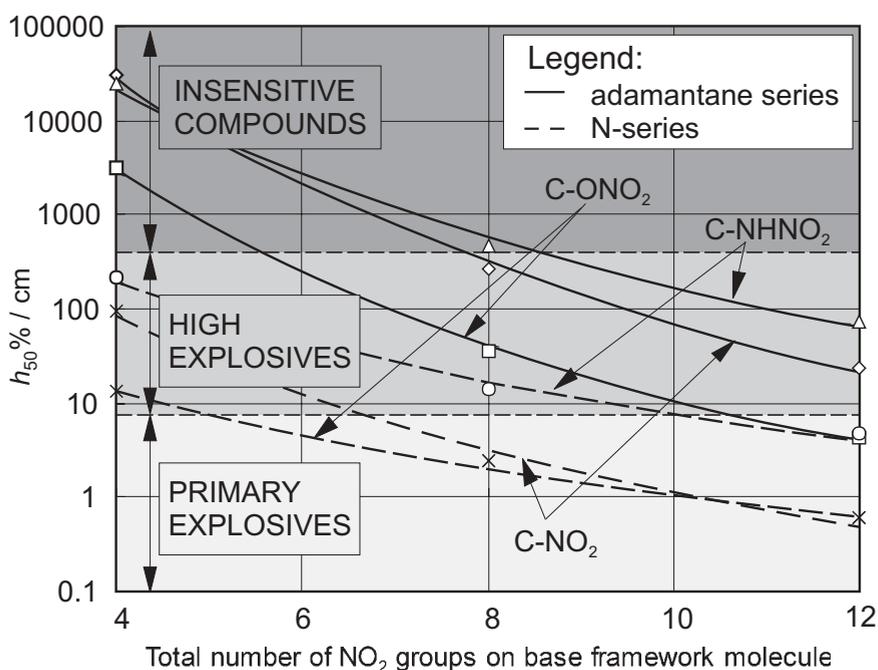


Figure 3. Dependence of impact sensitivity on total number of nitro groups on base framework.

From Figure 3 one can see that the same shape of dependence  $h_{50}\%$ -total number of nitrogroups is obtained for both series. At the same time, for the same degree of substitution, N-series derivatives are more sensitive than adamantane derivatives. This is a consequence of the higher  $OB_{100}$  value for the same degree of substitution.

It is important to note that sensitivities of adamantane derivatives were in the range of standard explosives, if eight (8) or more nitro groups were added, while nitroderivatives of N-series had sensitivities in the same range (of standard explosives) when only four (4) nitro groups were added. It is also evident that nitroderivatives of N-series with more than eight groups added become very sensitive – even more sensitive than some standard primary explosives.

It is known that, among polynitroaliphatic explosives having comparable oxygen balances, compounds containing at least one N–NO<sub>2</sub> linkage (called »trigger linkage«) are more sensitive than compounds containing only C–NO<sub>2</sub> linkages.<sup>7</sup> For the same degree of substitution in both of our series, C–ONO<sub>2</sub> compounds have higher oxygen balances than C–NO<sub>2</sub> and C–NHNO<sub>2</sub> compounds, and, as a consequence, higher sensitivities (Figure 3).

## CONCLUSIONS

Increasing the number of nitrogroups introduced on the basic molecule framework will increase the molecular mass of the obtained nitroderivatives, and consequently their densities. Such an increase of density will be most rapid for C–NO<sub>2</sub> nitroderivatives, and slowest for C–NHNO<sub>2</sub> compounds.

N-series nitroderivatives have higher densities (above 2 g cm<sup>-3</sup>) than their adamantane counterparts (the highest, 1.827 g cm<sup>-3</sup>). Considering this fact only, one might conclude that N-series nitroderivatives could be better energetic compounds. But, these compounds could have very high sensitivities. Calculated sensitivity values, even higher than the values of standard initial explosives, suggest a possible hazard in handling, and exclude them from possible synthesis, as well as from practical use. N-5 compound from N-series has an exceptionally high energy content, resulting from crowded NO<sub>2</sub> groups interactions. Interaction energy is 929 kJ mol<sup>-1</sup> and the calculated positive enthalpy of formation is 1183 kJ mol<sup>-1</sup>. These data make it thermodynamically less stable than its polynitroadamantane counterpart (DS-5).

Briefly, N-series nitrocompounds have higher densities and better detonation properties than nitrocompounds from the adamantane series. However, their high sensitivities suggest special precautions to be taken in their

possible synthesis. The same reasoning excludes them from possible use as high explosives.

Nitro compounds of the adamantane series mainly have calculated densities, sensitivities, and detonation properties like standard high explosives. For example, compound DS-5 with density of  $1.827 \text{ g cm}^{-3}$ , sensitivity  $h_{50}\%$ -24 cm, detonation velocity  $8372 \text{ m sec}^{-1}$  and detonation pressure 32.1 GPa would have better explosive characteristics than TNT, and in the range of pentrit and hexogen, respectively. In addition, its expected thermodynamic stability leads to the conclusion that DS-5 could be a potentially good high explosive.

Good explosive performances of polynitroadamantanes and the predictable low cost of their synthesis make them a very promising group of energetic compounds.

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### SAŽETAK

#### **Studij detonacijskih parametara polinitroadamantana, potencijalnih novih eksploziva. I. Odnosi molekularna masa/gustoća i bilanca kisika/osjetljivost**

*Danko Škare i Muhamed Sućeska*

Za različite polinitroadamantane i njihove alifatske analoge proučavani su odnosi molekulska masa/gustoća i bilanca kisika/osjetljivost te su izračunani neki eksplozijski parametri. Izračunane gustoće polinitroadamantana, kao i njihova osjetljivost i detonacijska svojstva, na razini su standardnih eksploziva. Neki od njih imaju čak bolja svojstva od TNT i slična su svojstvima pentrita i heksogena. Alifatski polinitro-analozi imaju veću gustoću i viši sadržaj energije, ali njihove izračunane visoke osjetljivosti na udar isključuju ih iz moguće upotrebe.