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STUDIES IN THE FIELD OF CHEMISTRY OF NITRO COMPOUNDS (TO 100TH BIRTHDAY ANNIVERSARY OF S. S. NOVIKOV)

Forecasting the Characteristics of the Explosives

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Abstract—The key techniques for forecasting of the properties of the explosives were presented. We acquired an array of the properties approximately for 200 explosives on the basis of literature information and own experimental data. Techniques of an evaluation of the main characteristics of the explosive transformation were developed. We forecasted properties of a series of compounds not synthesized earlier by computation methods. The experimental and computed data were combined into vast array of information approximately for 1000 explosives. The systematization of experimental data allows conclusions about the attained levels of efficiency and of safety, and also forecasting the properties of the promising explosives.

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In recent years a number of publications devoted to forecasting of the properties of explosives sharply increased. Among them there are works on some physicochemical characteristics of hypothetical structures [1, 2], and also ones where computed estimations of a set of energy parameters of the promising explosives are considered [3–5]. Very high forecast estimations for polynitrous compounds are given in a literature. For example, the prospects for the synthesis of tetrazatetranitrocubane, hexazadinitrocubane and other polynitrous compounds are explored among main directions of developments in the USA. The estimations of characteristics for the so-called "poly-nytrogens" are very high. For example, it was reported in [4] that detonation velocities in a range of 15–20 km s^{-1}, detonation pressure of 120–220 GPa, and missile force of more than 500% relative to octogen can be obtained. Long-term search of techniques for synthesis of octanitrocubane also was of ambitious prospects. The actually synthesized substance was of single crystal density by 0.2 lower than it was assumed but in this case all expectations for it lose meaning. It is assumed that the poly-nitrogen possesses both high density and heat of formation (about 5000 kcal kg^{-1}). These courageous expectations were suggested at computation of the properties of the explosives and thus superhigh computed values of the detonation parameters were obtained. In the case of use of a random approach to the search of new powerful explosives and substantiating the maximum possible capabilities on the one hand the forecast evaluations can testify for some reserves and on the other hand any guarantee that the best structure has found, practically is absent. Therefore system generalization of data on already synthesized and investigated explosives is required along with the forecasting of the properties of a wide range of the hypothetical structures at a further analysis of a relation of the main characteristics of the explosives.

The systematization of the properties of the explosives and the analysis of an effect of the chemical composition and structure on their main characteristics. The explosives are the wide range of the compounds which relate to different classes of chemical substances and prepared by different techniques. A rapid exothermic transformation with elimination of a large amount of gases as a result of an external action is their common capability. It is implied that the energy level of the external action is significantly lower than the thermal effect of decomposition.

A ratio of the energy of the external action and energy of decomposition determines the field of the explosive application. It should be emphasized that so-called insensitive explosives or explosives for an application in initiators along with the explosives with the maximum detonation parameters are the purpose of the search. The basic factor of system search is that the previously calculated estimation determines a direction of synthesis

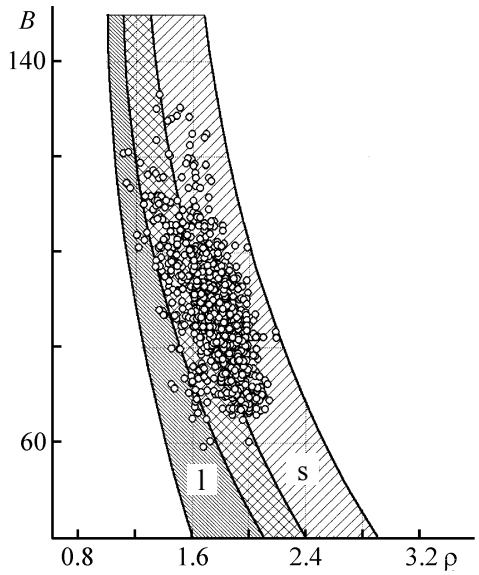


Fig. 1. Diagram ρ (g cm^{-3})–*B* (g-at kg^{-1}) for liquids (l) and solids (s). Points are district explosives; the same for Figs. 2, 3.

of the explosives with the given properties.

The preliminary estimating an applicability of the explosive for solving a concrete problem starts by computation of the main nonexplosive characteristics (if its have not found experimentally) such as the single crystal density, the heat of formation etc. An accuracy of their computation determines an accuracy of calculation of the detonation parameters and an operational safety. We used computation methods which assume the physicochemical characteristics as functions of the chemical structure of the explosives. It is reasonable to assert that all properties of substances are related to their composition and structure of molecules. Specifically, the structure determines three-dimensional distribution of the electron energy, strength of chemical bonds, dipole moments of molecules, reactivity of substances, a value of internal and intermolecular forces, also, as a whole the energy potential of molecule. A change in composition and structure of a matter leads to the regular response in the properties.

The fundamental regulation, that the explosives are not the separate class of chemical substances but they belong to the general set of chemical compounds, is one of the basic principles of the investigation. Motion inside this set cannot be arbitrary since it is accompanied by a completely single-valued change in the structure and it is interconnected with a composition change. The range of these changes is determined by limitations to existence of chemical bonds and valence states of entering elements.

We focused attention on the fact that is observed the sufficiently close relation between the density of substance and the specific summary content of gram-atoms in it (*B*). Last value is defined as the sum of atomic weights of all atoms in the formula, related to the molecular weight (or "formula weight").

Depicting diagram ρ–*V* (Fig. 1) was carried out with the use of data of chemical reference books (total number of points is about 900) with providing a maximum interval of the selected values. One of the remarkable properties of the represented diagram is the fact that it limits the region of existence of chemical substances, i.e., the parameters ρ and *V* cannot take arbitrary values for any substances. In accordance with Fig. 1 the regions of existence of liquids and solids partially overlap; however, chemical substances in these states of aggregation are absent out of the bounded space. Explosives are denoted on the diagram by points, their arrangement is also limited by a certain region which as already mentioned higher is the integral part of the totality. A change in the density and the formula weight is possible only in the case of some specified conditions. It is not possible to arbitrarily change the composition of substance since with a change in the number of gram-atoms of one element the well-defined change in the number of gram-atoms of other elements will occur. This relation is determined by the laws of the construction of molecules. Isomers are positioned in one region diagram and possess the close densities in the range of statistical straggling.

The fact that the relation of the characteristics of chemical composition and structure is general for the entire region of chemical substances, it allowed on sufficiently large array (including both explosive and nonexplosive substances) development of equations for computing the theoretical density of solid and liquid substances, and also for the heat of formation according to the atomic contributions. The methods of calculation of the density and enthalpy according to the atomic contributions are based on additivity of the molar volume and the enthalpy of formation relative to the sum of the atomic contributions. The system of the atomic contributions suggested in detail describes the structure of matter in the case of applying the additive diagrams for describing the relations of different properties with the composition and the structure. In general form it is possible to write that the specific volume of a gram mole of substance is equal to the sum of the volumes of the gram-atoms of its component with the correction for deformation in the cycles and in some groups atoms:

$$V_m = \sum_{K=C,N,O\ldots}^{n} \Sigma A_i K_i + \sum_{j=4}^{n} \Sigma C_j L_j + \Sigma D_k R_k, \quad (1)$$

where A_i is the contribution value of ith type of atoms (for instance, three type of atoms was examined for carbon: c_1 atoms with only single bonds; c_2 atoms with at least one double bond; c_3 atoms with a triple bond), K_i, number of ith gram-atoms in mole; C_j, correction value for cycles of jth order belonging to a molecule; L_j, number of the cycles of jth order in a mole; D_k, correction value for groups of kth type; R_k, number of group of kth type in a mole.

$$\rho = \mu/V_m, \quad (2)$$

where μ is weight of a mole.

The heat of formation can be computed analogously to the calculation of the specific volume of a mole (Eq. 1) (with the use of the corresponding coefficients A, C and R which denote the contribution forms of atoms to the energy content of a molecule).

Data which are concerned the explosive characteristics of individual substances are sufficiently disembodied. For example, there are sufficiently reliable data for the detonation velocity almost for two hundred of explosives (a data array comprising 425 lines for 185 solid and liquid explosives was form to determine interpolation dependences). Sensitivity to the mechanical actions according to the results of tests on pile drivers was evaluated approximately for 150 substances. However, the number of individual explosives for which both the characteristics of explosive transformation and sensitivity to various external actions are known, does not exceed hundred. Thereby there exist significant divergences in the properties reported in literature for the explosives most frequently utilized in the practical tasks or for research purposes. Therefore problem of evaluation of data reliability should be solved in the course of information accumulation. It should be noted that at generalization of information relative to any characteristic the evaluation of the data reliability was ambiguous, whereas at generalization of the basic properties of the explosives we considered the relationship of the group of properties for each explosive which significantly simplified the selection of correct value for each characteristic.

According to the method of experimental design the data array must be orthogonal and randomized (it must be kept a step for all used factors). These requirements at the array formation on the basis of the experimental data are physically unrealizable since among existing points we cannot select the points corresponding to the information complex and even close to it. If any point out of the examined area is regularly connected with it a motion over the response surface can occur only by an assigned way. Therefore extrapolation of the obtained dependences beyond boundaries of the examined area is controlled by their connections inside it.

The procedure "of the method of detecting the regularity" is sufficiently common and consists in the application of the regression analysis. The selection of the prevalent factors was carried out by the principle of inclusion and exclusion, a step regression with subsequent obtaining of interpolation dependences by several iterations and by removal after each of them culled data. Also the displacement of experimental data relating none to this statistics was conducted. This operation was carried out, as a rule, by several iterations developing new dependences and estimating accuracy by statistical methods after each step. The number of rejected results did not, as a rule, exceed 10–20%. For an increase in the accuracy of the equation the analysis of residuals for obtaining the validating regression equations was conducted.

The fundamental equations used for the evaluation of characteristics of the explosives are given below:
the calorimetric heat of explosion for the C, H, N, O-containing explosives (kcal kg^{-1})

$$Q_c = Q_{max}\, 4.261\rho^{0.291}(\Delta H_f + 1000)^{-0.261}\, a^{-0.107} b^{-0.012}\, c^{0.049} d^{0.072} + \Delta H_f; \quad (3)$$

the calorimetric heat of explosion for the C,H,N,O,F-containing explosives (kcal kg^{-1})

$$Q_c = Q_{max}\, 0.59\rho^{0.075}(\Delta H_f + 1000)^{0.018} a^{-0.063} c^{0.132} e^{0.027} + \Delta H_f, \quad (4)$$

where Q_{max} is maximum energy content of the explosion product (kcal kg^{-1}); ρ, density of the explosive (g cm^{-3}); ΔH_f, the heat of formation (kcal kg^{-1}); a, b, c, d, e, amount of gram-atoms of chemical elements in overall molecule (common formula $C_aH_bN_cO_dF_e$) of one kilogram (g-a kg^{-1});
number of moles of the gaseous products (mol kg^{-1})

$$N_r = 0.777\rho^{-0.153} B^{0.715}(\Delta H_f^0 + 1000)^{0.1} Q_{max.ex}{}^{0.238}, \quad (5)$$

where B is a sum of gram-atoms of chemical elements comprising one kilogram of the explosive; $Q_{max.ex}$, maximum heat of explosion (kcal kg^{-1});
the detonation velocity (km s^{-1})

$$D = 0.555\rho^{0.652}a^{-0.0039}c^{0.0764}\alpha^{0.0588} \times Q_{макс}^{0.231}N_{макс}^{0.120}, \quad (6)$$

where N_{max} is a number of moles of the gaseous products of explosion corresponding to the maximum heat of explosion (g mol kg^{-1}); α is coefficient of excess of an oxidizing agent (dimensionless);
the detonation pressure (gPa)

$$P = 3.4 \times 10^{-2}\rho^{2.022}a^{-0.0111}b^{0.00536}c^{0.149} \times Q_{max.ex}^{0.589}N_{max}^{0.260}; \quad (7)$$

A rate of expansion of a cylindrical shell caused by missile force of the sliding detonation products (m s^{-1})

$$W = 20.50\rho^{0.418}Q_c^{0.458}N_g^{0.245}\beta_E^{0.310}\Delta r^{0.1}, \quad (8)$$

where β_E is load coefficient ($\beta_E = m_E m_j^{-1}$, m_E, explosive weight, m_j, weight of the shell where the explosive was placed; $\Delta r = R - R_0$ (mm), R, R_0 are current and initial radii of the expanding tube.

An efficiency of the missile action according to technique M-60 relative to octogen (%)

$$\eta = 1.23\rho^{0.871}Q_c^{0.432}N_g^{0.230}; \quad (9)$$

critical pressure for a detonation initiation (GPa)

$$P_{cr} = (\rho B)^{2.732}Q_{max.ex}^{-1.534}\alpha^{-1.105} \times 1010^{-1} - 0.5; \quad (10)$$

the minimum diameter of the face (mm), under which detonation is transferred to the mass surrounding the explosive

$$d_{min} = (\rho B)^{1.696}Q_{max}^{-0.782}\alpha^{-1.275} - 10; \quad (11)$$

a critical thickness of the detonation (mm)

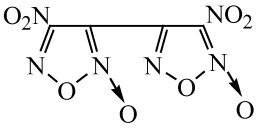
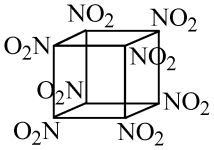
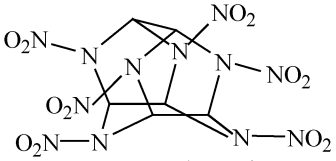
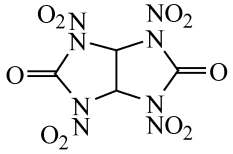
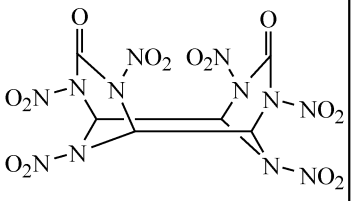
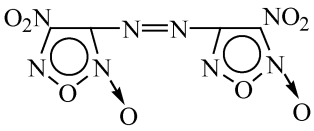
$$\Delta = (\rho B)^{1.264}Q_{max}^{-0.806}\alpha^{-0.171}\rho_{rel}^{1.409} - 1. \quad (12)$$

The complex calculation of energy and operating characteristics makes it possible to analyze the results, obtained for each distinct method, and to evaluate their applicability from the point of view of the explosive structure and composition. The possibility of the promising prognostication of the properties of new explosives is the basic reaching of this generalization

We systematized literary and own experimental data about for 200 explosives moreover we carried out data verification given by the different authors; and the missing information was augmented with data computed according to equations (3)–(12). An array fraction of the properties of the explosives described in the literature is listed in Tables 1, 2. The given in the tables properties of the explosives characterize both the reached efficiency and resistance to the shock-wave and mechanical actions. The results of the forecast of the explosive properties with the extremely high level of the energy density are presented in Table. 3. Besides for the comparison the properties of the standard explosives are listed in Tables 1–3. Designations in the tables and on the graphs are the same for equations (3)–(12). Furthermore, the sensitive to shock (SS) and to friction (SF) according to the results of testing on the pile drivers are presented in Table 1, 2: a higher resistance threshold to the shock, HT SS; the height, which corresponds to the fifty-percent probability of initiation, H_{50}; a higher resistance threshold to the friction, HT SF. All these characteristics are described in the literature.

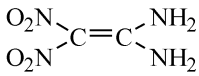
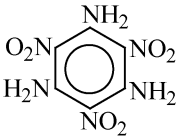
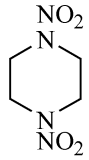
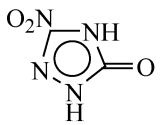
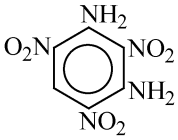
The development of equations (3)–(12) and others made it possible to produce the forecast calculation of properties for a range of the yet not synthesized compounds which nowadays are widely discussed (Table 3). The finally formed array contained experimental and calculation data about for 1000 explosives both of the investigated and hypothetical structures. The ranges of the variation of the properties in this array include all known at the present time high explosives. The ranking on the columns of their values was conducted to seek the extreme values of the main characteristics in the electronic table of the data array. For evaluating the reliability of the values that are forecasted for the hypothetical structures the analysis of the graphic dependences depicted on the basis of the data array was performed. The contour lines of the relative missile ability are represented in the axes of the density and content of nitrogen. The examination of the diagram allows conclusion that the maximum value of the relative missile ability does not coincide with the maximum content of nitrogen. Maximum relates to the content of nitrogen 34.0–46.0 g-at kg^{-1} that composes

Table 1. Brisant explosives

Comp. no.	Explosives	α	ρ_0, g cm^{-3}	ΔH_f^0	Q_c	D, km s^{-1} (at ρ_0)	P, gPa (at ρ_0)	η, %	P_{cr}, gPa	D_{min}	Δ	SS		SF HT, kgs cm^2
				kcal kg^{-1}						mm		HT	H_{50}	
1	hexagen	0.67	1.81	66	1330	8.60	32.7	96.7	2.05	10.0	0.48	70	160	2700
2	octogen	0.67	1.90	60	1320	9.11	36.1	100	2.4	16.0	0.70	70	85	2000
3	 dinitrodifuroxanyl	1.00	1.96	384	1730[b]	9.45[b]	43.9[b]	107.8[b]	0.2[b]	≤1[b]	0.03[b]	90[b]	200[b]	500[b]
4	 octanitrocubane	1.00	1.98	224	1738[a]	9.35[a]	39.0	108.2[a]	0.9[a]	2[a]	0.01[a]	10[a]	20[a]	2000[a]
5	 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaiso-wurtzitane (HNIW)	0.80	2.04	130	1400[a]	9.46[a]	42.8	105.9[a]	1.6[a]	15[a]	0.30[a]	50[a]	70	2500[a]
6	 sorgyl	1.03	2.03	18.0	1300	9.26	39.7	102	1.3	6	0.26	60[a]	70	2500[a]
7	 BK-6	1.00	2.07	–8	1380[a]	9.80[a]	42.5	105.7	1.2	8	0.2	20	30	500
8	$O_2NN[CH_2C(NO_2)_2NF_2]_2$ bisdifluoroaminodinitroethyl-nitroamine	1.25	2.04	–24	1490[b]	9.10[b]	40.7[b]	104[b]	0.3[b]	≤1[b]	<0.06[b]	50[b]	70[b]	850[b]
9	 azanitrofuroxan	1.00	2.00	554	1740[b]	9.70[b]	40.6[b]	110.3[b]	0.2[b]	≤1[b]	0.03[b]	60[b]	100[b]	500[b]

[a] Calculated value, [b] computation with data of [6, 7].

Table 2. Insensitive high power explosives

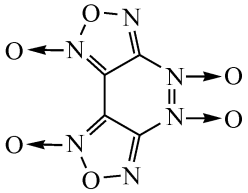
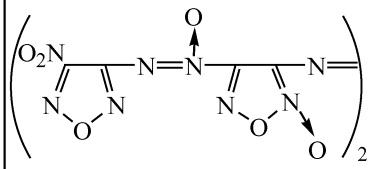
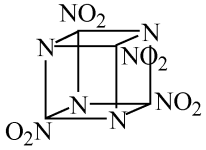
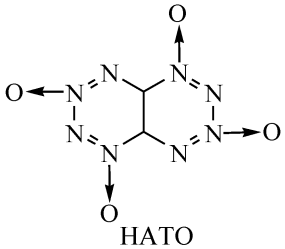
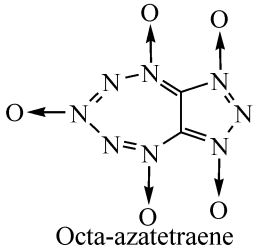
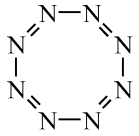
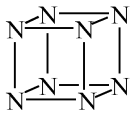
Comp. no.	Explosives	α	$\rho_{0,}$ g cm^{-3}	ΔH_f^0	Q_c	D, km s^{-1} (at ρ_0)	P, gPa (at ρ_0)	η, %	P_{cr}, gPa	D_{min}	SS		SF HT, kgs cm^{-2}
				kcal kg^{-1}					mm		HT	H_{50}	
1	hexogen	0.67	1.81	66.1	1330	$8.60_{(1.7)}$	96.7	2.05	10	0.48	70	160	2700
2	octogen	0.67	1.90	60.3	1320	$9.11_{(1.89)}$	100	2.4	16	0.70	70	85	2000
3	trinitrotoluene	0.36	1.66	–66.4	1000	$6.94_{(1.64)}$	76.4	4.2	>40	1.75	≥500	>500	6000
4	1,1-diamino-2,2-dinitroethylene (DADNE) 	0.67	1.89	–216	1164	8.61	92.6	4.2	31	0.68	180	120	4000
5	triaminotrinitrobenzene 	0.40	1.94	–154.8	933	7.95	86.0	7.3	>40	3.00	>500	200	8000
6	dinitropiperazine 	0.33	1.65	–72.7	1020	7.47	81.8	10.9	>40	1.71	>500	250	6000
7	HTO 	0.60	1.91	–205.5	929	8.27	83.8	5.2	>40	0.95	140	120	3000
8	triaminotrinitrobenzene (TATB) 	0.41	1.84	–112	900	$7.60_{(1.75)}$	82.8	5.3	>40	1.08	260	110	6000[a]

[a] Calculated value.

$\eta \approx 120\%$ (relative to the octogen with the density 1.875 on the speed of end throwing according to the technique M-60 [8]). In Fig. 2 the characteristics corresponding to octazacubane were not graphed because data for it presented in Table 3 were sufficiently approximate and validating of values of the density and the enthalpy of formation was required.

It should be noted that there exist the surface which corresponds to the average level of the explosive properties, composition and structure. In the three-dimensional coordinates the region limited by two surfaces is of the different thickness, which is also determined by the ratio of the composition and explosive structure. The region of existence is not continuous that is

Table 3. Computed data for hypothetical structures of the brisant explosives

Compd. no.	Explosives	α	ρ_0, g cm^{-3}	ΔH_f^0	Q_c	D, km s^{-1} (at ρ_0)	P, gPa (at ρ_0)	η, %	P_{cr}, gPa	D_{min}	Δ
				kcal kg^{-1}						mm	
1	hexagen	0.67	1.81	66	1330	8.60	32.7	96.7	2.05	10.0	0.48
2	octogen	0.67	1.90	60	1320	9.11	36.1	100	2.4	16.0	0.70
3	DPPDO 	0.75	2.02	568	1660	9.5	41.7	109 (119)[a]	0.8	8	>0.01
4	DN BAFS 	0.75	1.99	779	1750	9.7	42.7	110 (122)[a]	0.9	7	>0.01
5	TNTAC 	1.00	2.04	433	1680	9.9	44.7	110 (121)[a]	0.6	3	>0.01
6	OANT 	1.00	2.22	800	1680	10.7	55.0	120 (144)[a]	0.5	5	>0.01
7	HATO 	1.25	2.26	758	1600	10.8	53.0	119 (141)[a]	0.4	2	>0.01
8	Octa-azatetraene 	–	1.81	1476	1476	10.0	42.3	99 (98)[a]	0.4	2	0.05
9	Octa-azacubane 	–	2.28	1431	1431	9.9	52.0	115 (133)[a]	0.1	4	0.05
10	N_{20}	–	1.93	1331	1331	10.2	46.4	100.0	0.5	5	0.18

[a] The relative missile action computed by ratio of the energies is presented in the parantheses.

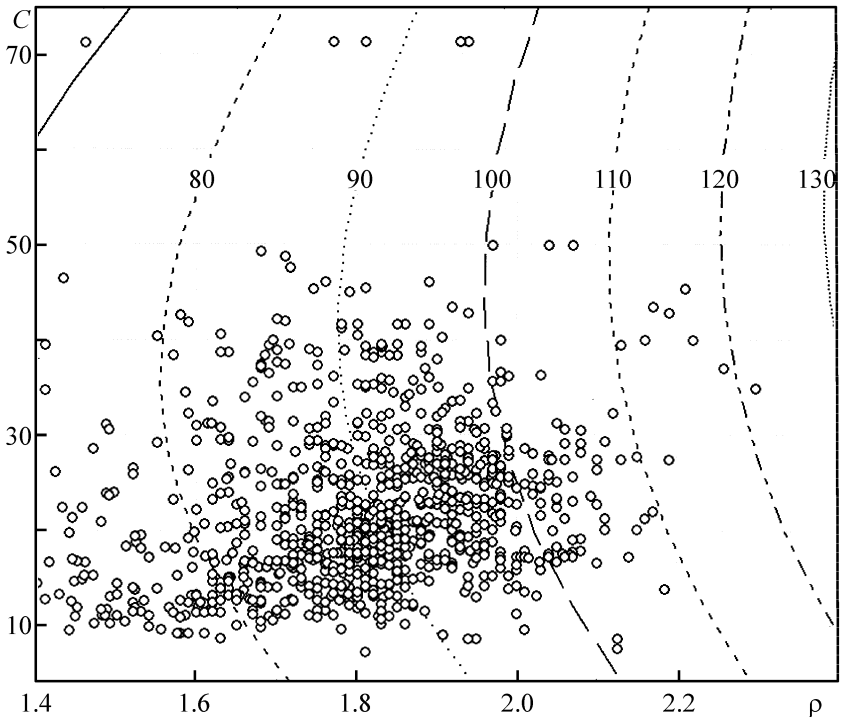


Fig. 2. Contour lines of the relative missile capability in geometry according to the M-60 techniques relative to octogen at the density 1.875 [8]. (ρ) density (g cm^{-3}), (*C*) number of gram-atoms per 1 kg of nitrogen. The appropriate values of the relative missile capability are pictured on the contour lines (%); the same on Fig. 3.

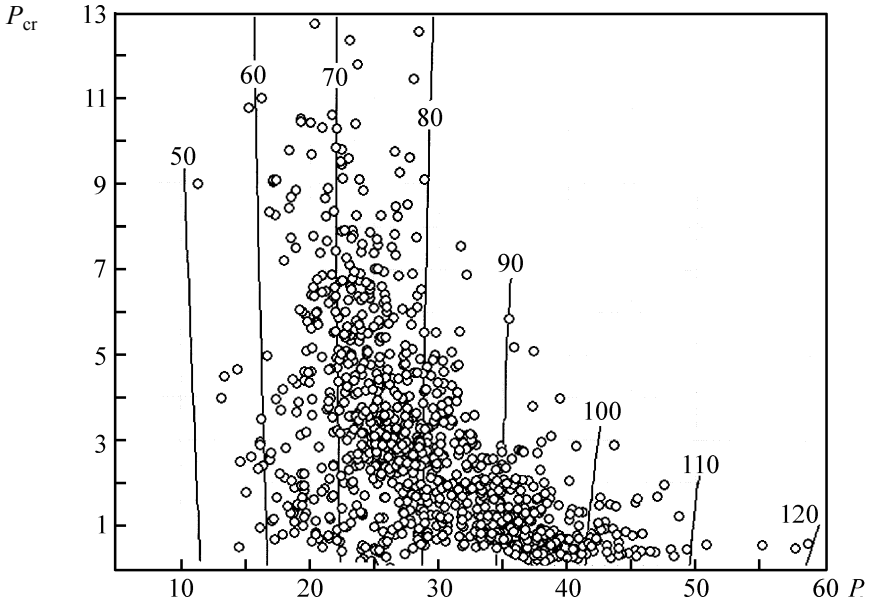


Fig. 3. Contour lines of the relative missile capability in geometry according to the M-60 techniques relative to octogen at the density 1.875 [8]. (*P*) the detonation pressure, gPa, (P_{cr}) the critical pressure of initiation, gPa.

connected with the chemical structure of a substance. The boundaries of the region of existence of the explosives are determined by an interaction of their composition and structure. Thus substances only with the parameters from the region of existence can be synthesized.

For the more evident explanation of the concept of the boundaries of the region of explosive existence we pictured the diagram of the contour lines of relative missile ability

η in the axes of the pressure of detonation and the critical pressure of the initiation P_{cr} (Fig. 3). Along the region of existence (Fig. 3) an increase in the energy content of the explosives leads to a growth of sensitivity to shock and friction. The indirect relation of the sensitivity and the energy content determine the boundaries of the region of existence. If the energy content value is lower than the certain critical value the substance becomes unexplosive. In accordance with Fig. 3 unexplosive substances can be limited by a bisector of quadrantal angle in the left upper angle. A supersensitive coompounds and chemically unstable substances correspond to the superhigh energy content. In Fig. 3 below the region of existence is limited by the X-axis passing through the zero value of the critical pressure. Note that a proposed maximum increase in the density and enthalpy of formation for the substances which are found on the boundaries of the region of existence additionally testifies about the low chemical stability of such molecules. Synthesis of the substances which have simultaneously high knock ratings and low sensitivity is impossible. In this case as it follows from equations (7)–(10), a relative increase in the sensitivity of the explosives with an increase in the energy content Q_{max} considerably anticipates a relative increase in the detonation parameters and characteristics of the explosive efficiency

In the course of consideration of the experimental and computed values of the explosive characteristics in the entire region of existence we performed verification and suggested certain ideas about features of the probable search of the substances with the maximum characteristics.

CONCLUSIONS

(1) We obtained the explosives with the density of a single crystal 2.0–2.07 g cm^{-3}, the heat of explosion approximately 1750 kcal kg^{-1}, the detonation pressure 40–45 gPa, the pulse of missile action about 104–108% (relative to the octogen). However, the level of sensitivity to shock and friction is significantly higher than in the standard substances. The most acceptable substance HAV has the sensitivity near the level of PETN (pentaerythrityl tetranitrate). For their preparation, processing, and operation a large number of preventive measures should be developed and realized to reduce the risk in dealing with the explosives.

(2) The analysis of the dependence of the explosive properties on their composition and structure allow assertion that preparation of the explosives with the indices which exceed the attained values is possible. The region of the elemental compositions for the explosives with the extreme characteristics places within the limits $C_{2-5}N_{52-68}O_{2-10}$ (hydrogen is absent). The attainment of the density of a single crystal 2.0–2.3 g and the enthalpy of formation approximately 500–1500 kcal kg^{-1} is possible for selected explosives. This allows reaching the values of the heat of explosion 1800–1850 kcal kg^{-1}, the pressure of detonation 50–60 gPa and the pulse of missile action 115–125% (relative to octogen). All substances with such high parameters have the unacceptable level of safety: the critical pressure of the initiation of detonation 1.5–5 kbar and less, the critical thickness of detonation from 1–10 μm to 50 m. Nowadays the measures to reduce the risk in dealing with these explosives are unknown.

The carried out estimation of the properties of the allotropes of nitrogen of various structures as high energy materials allows conclusion that the most probable result is preparation of substances with the density 1.4–2.0 g cm^{-3}, the enthalpy of formation (the heat of explosive transformation), 1300–1620 kcal kg^{-1}, the pressure of detonation, 40–50 gPa, the pulse of missile action, 100–115%. The sensitivity of these compounds is superhigh.

REFERENCES

1. Pivina, T.S., Molchanova, M.S., Korolev, V.L. et al., Abstracts of Papers, *35th Int. Pyrotec. Sem. Fort Collins*., Colorado. USA., 2008, pp. 277–291.
2. Nechiporenko, G.N., Lempert, D.B., and Soglasnova, S.I., *New Trends in Research of Energetic Materials,* Czech Republic, 2008, pp. 694–705.
3. Pepekin, V.I. and Gubin, S.A., *FGV*, 2007, vol. 43, no. 1, pp. 99–111.
4. Henric, Ostmark, *New Trends in Research of Energetic Materials,* Czech Republic, 2006, pp. 231–250.
5. Talavar, M.B., Sivabalan, R., Astana, S.R., and Singkh, Kh., *FGV*, 2005, vol. 41, no. 3, pp. 29–45.
6. Litvinov, B.V., Fainzil'berg, A.A., Pepekin, V.I., et al., *Dokl. Akad. Nauk*, 1994, vol. 336, no. 1, pp. 67–68.
7. Pepekin, V.I., Kostikova, L.M., and Lebedev, V.P., Abstracts of Papers, *36th Int. Conf. ICT 32, Int. Pyrotec. Sem.,* 2005, Karlsruhe, P. 95.
8. *Metody issledovaniya svoistv materialov pri intensivnykh dinamicheskikh nagruzkakh* (Methods of Investigation of Properties of Materials at Intensive Dynamic Loads), Zhernokletov, M.V., Ed., Sarov, 2005.