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Energetic Potential of Compositions Based on High-Enthalpy Polynitrogen Compounds

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An analysis is performed of the energy properties of solid high-energy systems containing ultrahigh-enthalpy polynitrogen compounds as the only component and in combination with other substances required to produce compositions with necessary operational characteristics. Special attention is given to the restriction of the combustion temperature by introducing substances with a high hydrogen content and a binder into the compositions. Such systems are compared with the best versions of real energetic compositions. As examples, calculations are given for compositions containing both hypothetical compounds (tetraazatetrahedrane N_4, octaazacubane N_8, trioxyhexazine N_6O_3, etc.) and real (derivatives of pyrroles, pyrazoles, triazoles, tetrazoles, and other polynitrogen high-enthalpy compounds).

Key words: specific impulse, combustion temperature, energetic compositions, enthalpy of formation, polynitrogen compounds, oxidizers.

INTRODUCTION

In recent 10–15 years, considerable progress has been made in the theoretical and experimental chemistry of high-energy compounds superior in detonation velocities to conventional explosive materials. Numerous quantum-chemical calculations have been performed for a number of compounds, including hypothetical ones, whose high enthalpies of formation and densities are achieved by creation of stressed structures consisting almost only of nitrogen atoms [1–7] or containing, in addition to nitrogen, N-oxide oxygen, which is introduced into molecules for stabilization. Significant advances have also been made in the chemistry of high-enthalpy polynitrogen heterocycles, in which the fraction of carbon atoms is successively reduced. In addition to the prospects of using these compounds as powerful explosives, many authors consider such ultrahigh-enthalpy compositions to be very promising in rocket engineering [8–13]. Of course, most of the currently proposed ultrahigh-enthalpy hypothetical compounds and those consisting of only one nitrogen will never be synthesized, but it is not impossible that some compounds of this class will nevertheless be produced.

A major drawback of studies searching for new high-nitrogen energetic compounds is an inadequate analysis of the energy potentials of individual representatives of such compounds. It is not taken into account that, in addition to the main energy carrier, important contributions to the energy potential comes from the other compounds introduced into compositions to sustain a number of required parameters other than energetic ones. For example, in designing compositions, it is very important to take into account that the combustion temperature should not be very high since the higher its excess over the values 3800–4000 K, the higher the heat loss to the walls of structures and the entire gain in real energetics can be nullified. Unduly optimistic projections are associated with the production of propellant compositions based on ultrahigh-power energetic compounds superior in energetics to known compositions or those which have not been, but could be, synthesized. Excessive optimism leads to an unreasonably elevated interest in some directions in the chemistry of high-energy materials and some chemical compounds whereas there are more promising alternatives.

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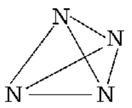
TABLE 1

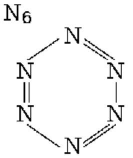
Properties of Hypothetical Nitrogen Structures [14]

No.	Substance	ρ, g/cm^3	ΔH_f^0		Detonation velocity km/sec
			$\frac{\text{kcal}}{\text{mole}}$	$\frac{\text{kcal}}{\text{kg}}$	
1	N_4	1.75	268.7	4800	13.24
2	N_6	1.97	345.6	4100	14.04
3	N_8	2.15	406.7	3650	14.86
4	N_{10}	2.21	473.4	3400*	12.08
5	N_{60}	2.67	546	650	17.31

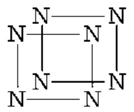
No. 1. N_4



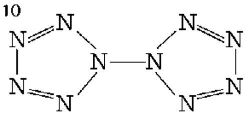
No. 2. N_6



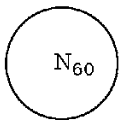
No. 3. N_8



No. 4. N_{10}



No. 5. N_{60}



Note. The value of ΔH_f^0 marked by an asterisk is highly overestimated. From our estimates of the enthalpy contribution of the substitution of the $>$ N— group for the $>$ CH— group and formation of a bicycle with a $>$ N—N $<$, bond, the enthalpy of formation of bipentazole is close to +1850 kcal/kg.

The present paper analyzes the energy properties of solid energetic compositions in which ultrahigh-power energetic substances, primarily hypothetical ones, with very high enthalpies of formation are included as individual components or in combination with other components. The compounds considered are compared with the best versions of propellant compositions based on real compounds.

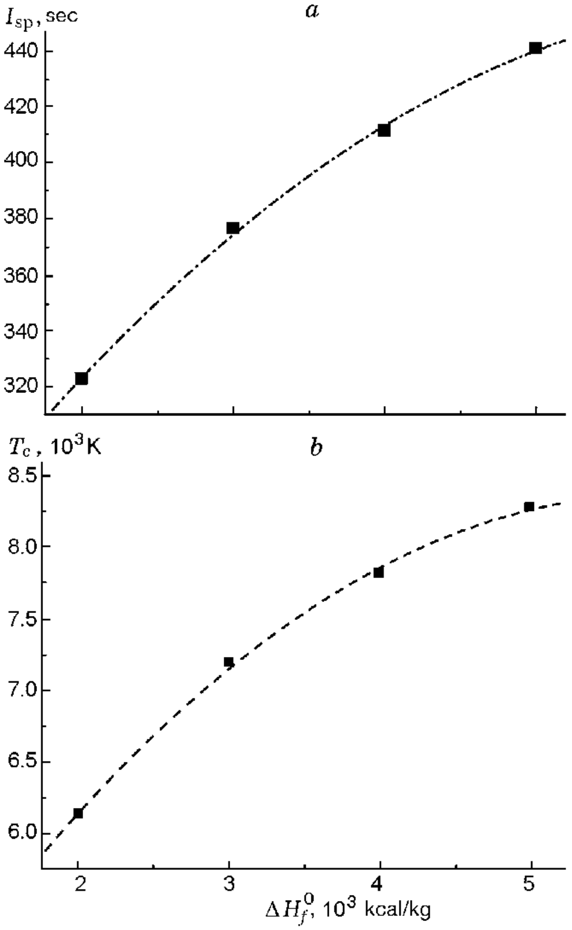


Fig. 1. Specific impulse (a) and temperature (b) of 100% N_x rocket propellant in a combustion chamber versus the enthalpy of formation.

THERMODYNAMIC COMPUTATIONAL-ANALYTICAL STUDIES AND DISCUSSION OF RESULTS

Among the abundance of hypothetical polynitrogen structures proposed in the literature, those mentioned in [14] and presented in Table 1 are of particular interest. Of course, the enthalpy of formation (ΔH_f^0) and density cannot be obtained with accuracy to the third or fourth decimal place; therefore, in the present calculations of the energy properties of rocket propellants, the density values were rounded to the second decimal place and the heat of formation to 50 kcal/kg.

Thermodynamic calculations of the specific impulse I_{sp}, combustion chamber temperature T_c, and nozzle exit temperature T_a were performed using the TERRA software [15]. It was assumed that the combustion chamber pressure was $p_c = 40$ atm and the nozzle exit pressure $p_a = 1$ atm.

Before proceeding to concrete high-nitrogen compounds, it is necessary to estimate the energy potential of these compounds as a function of the enthalpy of formation. Figure 1 gives calculated data for a composition containing the only component N_x. The dependence of I_{sp} and T_c on ΔH_f^0 can be approximated by the equations

$$I_{\text{sp}} = 185 + 0.0813\Delta H_f^0 - 6.0750 \cdot 10^{-6}(\Delta H_f^0)^2, \quad (1)$$

$$T_c = 3232 - 1.76\Delta H_f^0 - 1.507 \cdot 10^{-4}(\Delta H_f^0)^2, \quad (2)$$

which accurately (with a deviation not higher than 2 sec for $I_{\rm sp}$ and 40 K for T_c) describe calculated data for $2000 < \Delta H_f^0 < 5000$ kcal/kg (see the curves in Fig. 1). At $p_c : p_a = 40:1$, the quantity $I_{\rm sp}$ reaches 275 sec even for $\Delta H_f^0 \approx 1400$ kcal/kg. For $\Delta H_f^0 > 3000$ kcal/kg, the value of $I_{\rm sp}$ exceeds 360 sec, which is currently considered extremely high. However, even for $I_{\rm sp} = 275$ sec, the combustion temperature is already higher than 4600 K. Hence, to reduce the value of T_c, it is necessary to introduce additional components into the composition. In most cases, a decrease in T_c will be accompanied by a decrease in $I_{\rm sp}$, and, hence, a major goal of the study should be to find systems in which a decrease in T_c is accompanied by the lowest losses in $I_{\rm sp}$.

Another step in the development of the problem posed was an investigation of binary mixtures containing a high-enthalpy compound N_x and a second component as a promising mass carrier. This composition can contain much hydrogen, nitrogen or even lithium, which, in the absence of halogens at high temperatures, is primarily in the form of a monatomic gas. An explanation of the fact that, with high enthalpies of formation of the high-nitrogen component, an increase in the fraction of the second component, for example, LiH, to a certain value can be accompanied by an increase $I_{\rm sp}$ (Fig. 2) is that, at very high temperatures, an increase in the fraction of the mass carrier (mole/kg) is more favorable than an increase in the heat effect. Table 2 shows the values of the content of the second component for which the temperature T_c decreases to 4000 K for a given ΔH_f^0 of the polynitrogen energetic component and the corresponding values of $I_{\rm sp}$. The calculations were performed for systems in which the second component was lithium hydride, metallic lithium, hydrazonium azide ($N_2H_5N_3$ and $\Delta H_f^0 = +785$ kcal/kg), and a mixed salt of hydrazonium azide with triaminoguanidine azide [$C(NH{-}NH_2)_3N_3 \cdot N_2H_5N_3$; $\Delta H_f^0 = +630$ kcal/kg]. Figure 3 illustrates the results obtained. It is evident that, at $T_c < 4000$ K, the best second components are LiH, $N_2H_5N_3$, and $CN_{14}H_{14}$. Metallic lithium is slightly inferior to them at not too high values of ΔH_f^0 of the polynitrogen component. We note that to decrease T_c to 4000 K, it is necessary to add 25% LiH and Li to the composition (for $\Delta H_f^0 \approx +4000$ kcal/kg), whereas if $N_2H_5N_3$ or $CN_{14}H_{14}$ are used for this purpose, the latter already prevail in the composition.

Next, we consider compositions containing a binder. Of course, any real binder introduced into such a composition will reduce T_c. In the present work we study compositions containing three radically different types of model binder: hydrocarbon based binder (HCB, $CH_{1.67}$, $\Delta H_f^0 = -94$ kcal/kg, and density 0.91 g/cm^3); a binder with a large number of nitro groups [so-called active binder (AB), $C_{18.96}H_{34.64}N_{19.16}O_{29.32}$, $\Delta H_f^0 = -181$ kcal/kg, and density 1.49 g/cm^3] and an intermediate version — polyvinyl diazenoxide (PVDO, $C_3H_6N_2O_2$, $\Delta H_f^0 = -14$ kcal/kg, and density 1.31 g/cm^3). Since the densities of these binders are greatly different, their mass fractions are taken to be equal to 13, 20, and 17%, respectively, in order that the volume fraction of the binder in the compositions is approximately identical and close to a value that allows a technological processing of the energetic mass. Setting $\Delta H_f^0 =$ 2000–5000 kcal/kg for the main energetic component N_x, for compositions with all binders with their indicated content, we have $T_c > 4000$ K except for the composition 13% HCB + 87% N_x (+2000 kcal/kg), for which T_c is slightly lower than 4000 K. By increasing the binder content, it is possible to further reduce T_c, but this will considerably reduce $I_{\rm sp}$ (Fig. 4 gives an ex-

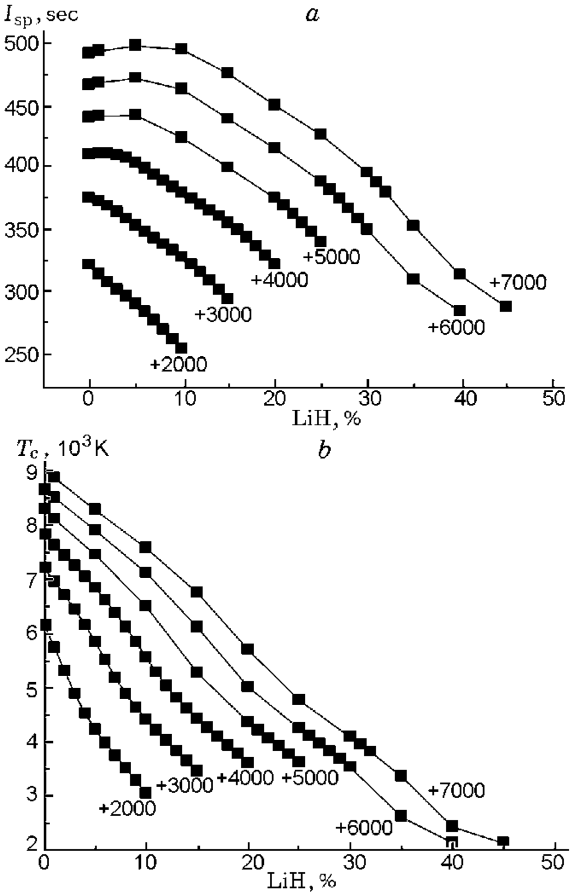


Fig. 2. Specific impulse (a) and temperature (b) of rocket propellants of composition $N_x +$ lithium hydride in a combustion chamber versus the enthalpy of formation of N_x and content of lithium hydride.

TABLE 2

Content of the Second Component for Maintaining Temperature $T_c \leqslant 4000$ K
and the Corresponding Value of I_{sp}
for a Given ΔH_f^0 of the Polynitrogen Component

ΔH_f^0, kcal/kg	Second component of composition							
	LiH		Li		$N_2H_5N_3$		$CN_{14}H_{14}$	
	C, %	I_{sp}, sec	C, %	I_{sp}, sec	C, %	I_{sp}, sec	C, %	I_{sp}, sec
2000	5.87	286.0	9.75	276.6	29.15	296.6	26.75	290.9
3000	12.04	316.6	18.70	299.3	48.25	319.4	45.2	311.7
4000	17.54	340.8	26.10	316.5	59.25	331.6	56.25	323.7
5000	22.40	360.7	32.20	330.0	66.40	339.2	63.7	330.9
6000	26.72	377.5	37.42	341.5	71.50	344.5	69.0	336.0
7000	30.60	391.8	41.87	350.8	75.23	348.4	72.8	339.9

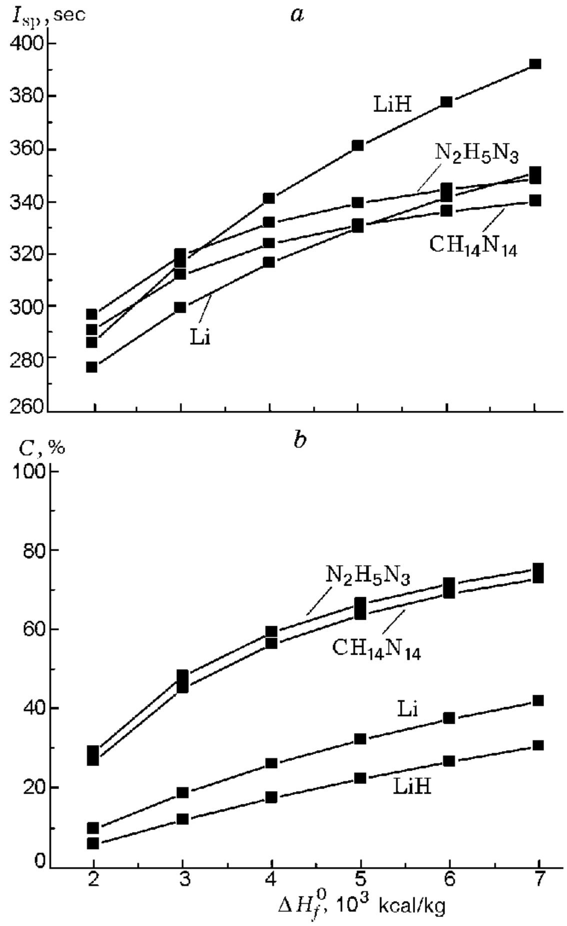


Fig. 3. Specific impulse for compositions N_x + second component (T_c=4000 K) versus the enthalpy of formation of the polynitrogen component (a) and the fraction of the second component (b) required to satisfy the condition $T_c = 4000$ K.

TABLE 3

Comparative Characteristics of Some
Real Energetic Compositions

Composition	I_{sp}, sec ($p_c : p_a = 40 : 1$)
Be + ADNA (NH_4 $N(NO_2)_2$) + HCB	282
BeH_2 (26%) + $N_2H_5N(NO_2)_2$ (74%)	318
AlH_3 + AB + ADNA	275
Al + ADNA + HCB	262
$H_3B \cdot H_2N$—$NH_2 \cdot BH_3$ (100%)	278
$B_{10}H_{14}$ (45%) + $N_2H_5N_3$ (55%)	293
Al + HCB + NH_4ClO_4 + HMX	256
Al + HCB + NH_4OClO_4 + HMX	262

ample for binder $+ N_x$ systems, $\Delta H_f^0 = 3000$ kcal/kg). Figure 5 shows the values of I_{sp} (at $T_c \leqslant 4000$ K) that can be reached when using the above-mentioned binder. However, the problem of decreasing T_c in compositions with binders can be solved more successfully by keeping the fraction of the binder not higher than the quantity sufficient for processing of the mass but with the addition of another gas-generating component, for example, hydrazonium azide. This solution also leads to a decrease in I_{sp} although this decrease is smaller. Figure 6 shows what values of I_{sp} can be reached by this method and what fractions of hydrazonium azide are required for this. It is evident that, with such different binders, there is no large difference in the achievable value of I_{sp}. In systems that do not have a binder but only contain the amount of hydrazonium azide that is required to satisfy the condition $T_c \leqslant 4000$ K, the values of I_{sp} are only 5–6 sec higher and are reached for a much larger amount of hydrazonium azide.

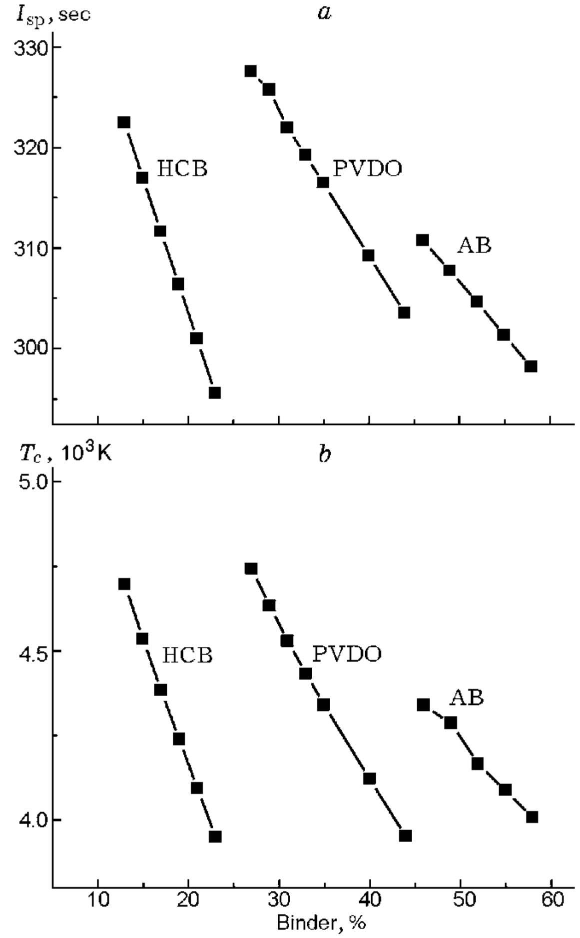


Fig. 4. Parameters I_{sp} and T_c of N_x + binder systems ($\Delta H_f^0 = 3000$ kcal/kg) versus the nature of the binder and its content.

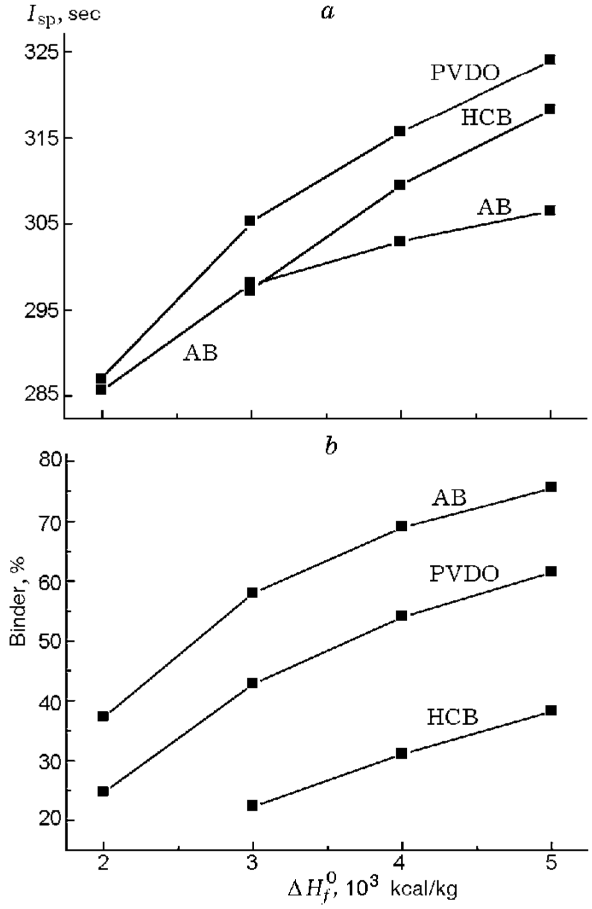


Fig. 5. Specific impulse for N_x + binder systems ($T_c \leqslant 4000$ K) versus the enthalpy of formation of the energetic component N_x (a) and the binder content (b) required to satisfy the condition $T_c \leqslant 4000$ K.

Thus, it can be stated that for solid energetic propellant compositions based on high-enthalpy compounds N_x for $T_c \leqslant 4000$ K and $p_c : p_a = 40 : 1$, the maximum achievable values of I_{sp} are equal to approximately 290, 310, 320, and 330 sec for the polynitrogen component with $\Delta H_f^0 = 2000$, 3000, 4000, and 5000 kcal/kg, respectively, and for any energetic component N_x with $\Delta H_f^0 = 2000$–5000 kcal/kg, the approximate limiting level of the specific impulse I_{sp} is the one that can be obtained in a solid composition, in practice, namely

$$I_{sp,\,max} = 234 + 0.342 \cdot \Delta H_f^0 - 3 \cdot 10^{-6} \cdot (\Delta H_f^0)^2. \quad (3)$$

Using Eqs. (1)–(3), it is easy to estimate that tetraazatetrahedrane N_4 (substance No. 1 in Table 1) as a monopropellant gives the value $I_{sp} = 435$ sec at $T_c = 8200$ K, whereas in the composition with a binder and a gas-generating component at $T_c \leqslant 4000$ K, it is impossible to obtain I_{sp} in excess of 330 sec. For octaazacubane N_8 (No. 3 in Table 1), these quantities are equal to $I_{sp} = 401$ sec at $T_c = 7650$ K against $I_{sp} = 319$ sec at $T_c = 4000$ K, and for bipentazole N_{10} (No. 4 in Table 1 with $\Delta H_f^0 = 1850$ kcal/kg), $I_{sp} = 314$ sec at $T_c = 5960$ K against $I_{sp} = 287$ sec at $T_c = 4000$ K.

For comparison, Table 3 gives values of I_{sp} for high-impulse compositions based on real compounds. It is evident that the level of $I_{sp} \geqslant 310$ sec (which could be achieved on the basis of solid N_x with $\Delta H_f^0 \geqslant 3000$ kcal/kg) is far superior to that of all available compositions.

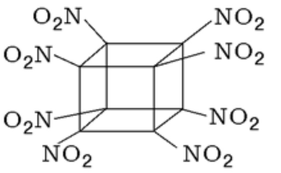
Since it is extremely improbable that high-enthalpy compounds having the minimum stability as energetic components can be produced on the basis of only nitrogen atoms, we will consider more real, though not so high-enthalpy, compounds which, in addition to a large amount of nitrogen, contain carbon atoms, hydrogen,

TABLE 4

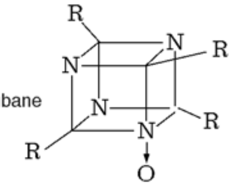
Energy Properties of Compositions Based on Some High-Enthalpy Compounds ($p_c : p_a = 40 : 1$)

No.	Main component (ΔH_f^0 kcal/kg; ρ, g/cm^3)	Binder	$I_{\rm sp}$, sec	ρ, g/cm^3	T_c, K
1	Octanitrocubane ($C_8N_8O_{16}$) [12] (+390; 1.979)	12% HCB	268.5	1.77	3770
		14% PVDO	265.7	1.85	3800
2	Tetranitrotetraazacubane ($C_4N_8O_8$) R = NO_2 (+660; 2.19 [16])	9% HCB	272.6	1.94	3860
		10% HCB	271.4	1.92	3810
		14% PVDO	270.7	2.00	3860
		16% AB	264.6	2.04	3830
3	Tetranitrotetraazacubane dioxide ($C_4N_8O_{10}$) (+ 560; 2.19)	10% HCB	273.2	1.92	3830
		16% PVDO	267.6	1.98	3790
4	Tetranitrotetraazacubane tetroxide ($C_4N_8O_{12}$) (+450; 2.19)	10% HCB	270.3	1.92	3780
		18% PVDO	264.1	1.95	3720
5	Octaazacubane tetroxide (N_8O_4) (+1650; 2.10)	10% HCB	302.0	1.86	4300
		12% HCB	305.4	1.82	4280
		15% HCB	309.3	1.76	4240
		12% PVDO	287.1	1.96	4160
6	Trioxyhexazine (N_6O_3) (+780; 1.80)	13% HCB	271.7	1.60	3680
		22% PVDO	262.1	1.66	3570
		30% PVDO	269.0	1.62	3595

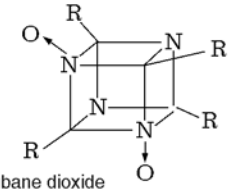
No. 1. $C_8N_8O_{16}$
Octanitrocubane



No. 2. $C_4N_8O_8$
Tetranitrotetraazacubane
R = NO_2

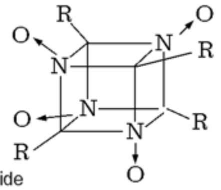


No. 3. $C_4N_8O_{10}$



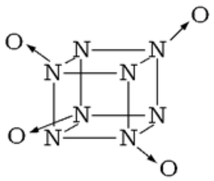
Tetranitrotetraazacubane dioxide

No. 4. $C_4N_8O_{12}$

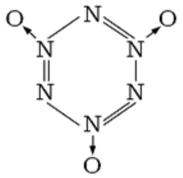


Tetranitrotetraazacubane tetroxide

No. 5. N_8O_4
Octaazacubane tetroxide



No. 6. N_6O_3
Trioxyhexazine



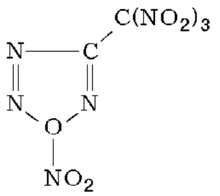
oxygen, and fluorine. These can be series of chemical compounds based on pentatomic (azoles) and hexatomic (azines) cycles and skeleton structures, where in each series, the carbon atoms in a cycle or skeleton are gradually replaced by nitrogen atoms. The functional groups at carbon atoms can be —H, —NH_2, —N_2H_3, —N_3, —NO_2, —NH—NO_2, —N_2, —$C(NO_2)_3$ and others that function as an oxidizer or a mass carrier. A combination of these groups can provide the optimal use of the energetic potential in a particular heterocycle or skeleton. Table 4 gives calculated values of $I_{\rm sp}$ and T_c, and density of energetic compositions based on some similar compounds.

TABLE 5

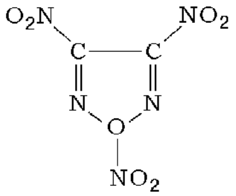
Energy Characteristics of Some Systems with a Binder

No.	Main component (ΔH_f^0, kcal/kg)	Binder	I_{sp}, sec	T_c, K
1	$C_2N_8O_8$ (+307*)	11% HCB	258.8 [18]	3560
2	$C_2N_6O_6$ (+340*)	11% HCB	258.0 [18]	3560
3	$C_4N_6O_8$ (+360 [19])	10% PVDO	261.4	3690
4	$C_6N_{12}O_{16}$ (+395*)	12% HCB, 20% PVDO,	265.2 262.5	3660 3680
5	$C_6N_{12}O_{10}F_2$ (+430*)	12% HCB 18% PVDO 20% AB	268.4 276.3 270.5	3780 3970 3910
6	$C_4H_2N_{10}O_8$ (+335*)	18% PVDO 20% AB	269.2 266.4	3690 3690
7	$C_2N_5O_4F$ (+335 [17])	16% PVDO 20% AB	265.3 259.9	3740 3700

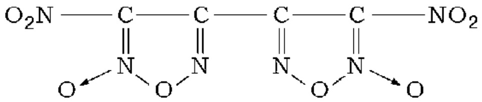
No. 1. $C_2N_8O_8$



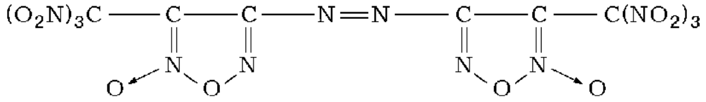
No. 2. $C_2N_6O_6$



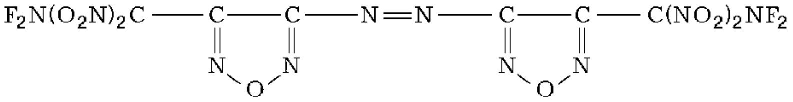
No. 3. $C_4N_6O_8$



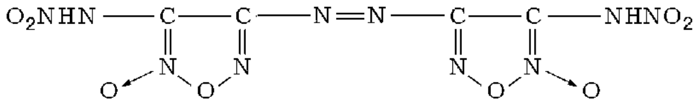
No. 4. $C_6N_{12}O_{16}$



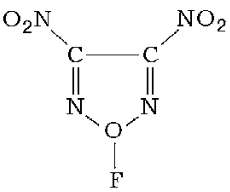
No. 5. $C_6N_{12}O_{10}F_2$



No. 6. $C_4H_2N_{10}O_8$



No. 7. $C_2N_5O_4F$



Note. The values of ΔH_f^0 marked by an asterisk were estimated taking into account the replacement of part of the fragments in compounds of close structure [17, 19, 20] with known value of ΔH_f^0.

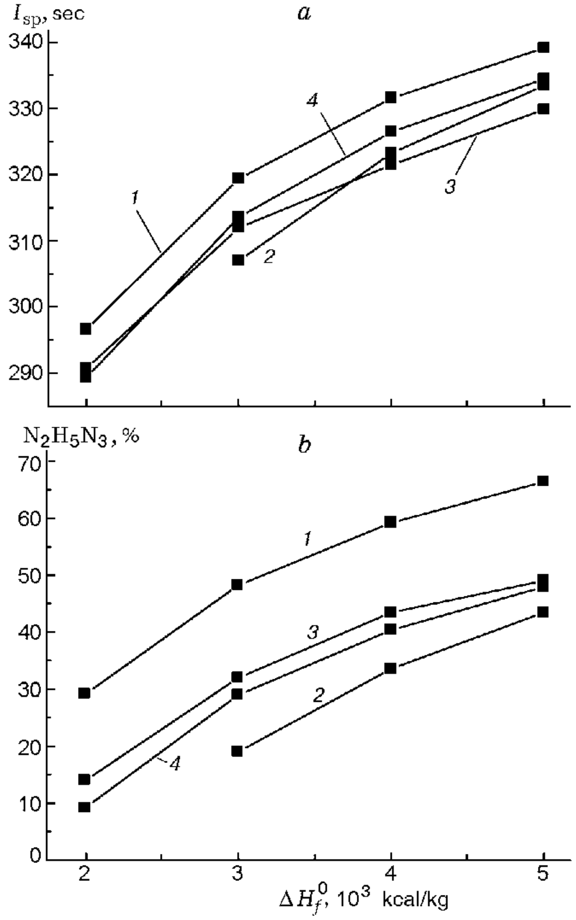


Fig. 6. Specific impulse I_{sp} in N_x + binder + hydrazonium azide systems ($T_c = 4000$ K) versus the enthalpy of formation of N_x (a) and the mass fraction of hydrazonium azide (b) required to decrease T_c to 4000 K: 1) without binder; 2) with HCB; 3) with AB; 4) with PVDO.

Preliminary estimates have shown compounds designed using polynitrogen high-enthalpy heterocycles can provide the level of $I_{sp} = 290$–300 sec. Although this is markedly inferior in energetic potential to the polynitrogen structures with 100% nitrogen content considered above but is considerably superior to compositions based on known oxidizers of available high-energy systems, except for compositions based on beryllium hydride. Table 4 gives calculation data on some N-oxides of polynitrogen energetic compounds (see Nos. 5 and 6). Such N-oxides can be more accessible than the initial structures with 100% nitrogen content, since, according to quantum-chemical calculations, the N-oxide oxygen stabilizes the molecule [14]. However, the values of ΔH_f^0 of N-oxides are much lower and this loss in the value of ΔH_f^0 cannot be compensated for by introducing oxygen in the molecule.

A combination of an increased content of high-enthalpy nitrogen, NO_2 type oxidizer groups, and carbon atoms in one molecule considerably stabilizes the compound but leads to a sharp decrease in the value of ΔH_f^0 and, hence, I_{sp} (Table 5). However, based on such compounds, it is possible to create compositions with high values of I_{sp} and quite acceptable values of T_c. In this case, compositions based on compounds with those high enthalpies of formation do not require additional aluminum [21], which increases only the temperature T_c without affecting the value of I_{sp} and frequently even decreasing it.

CONCLUSIONS

Hypothetical stressed polynitrogen compounds with an enthalpy of formation $\Delta H_f^0 > 2000$ kcal/kg have a very high energetic potential. Used as monocomponents for $\Delta H_f^0 = 4000$ kcal/kg and $p_c : p_a = 40 : 1$, they provide values of $I_{sp} = 320$ sec or higher, up to 400 sec. The high values of I_{sp} are accompanied by extremely high combustion temperatures (above 6000 K even at $\Delta H_f^0 > 2000$ kcal/kg).

In combination with components rich in mass carrier, these compounds can provide specific impulse in the range $I_{sp} = 290$–360 sec at $T_c \leqslant 4000$ K, depending on their enthalpy of formation.

In combination with various binders and components rich in mass carrier, under the same condition ($T_c \leqslant 4000$ K), it is possible to reach values $I_{sp} = 290$, 310, and 320 sec for a value of ΔH_f^0 of the polynitrogen component equal to 2000, 3000, and 4000 ckal/kg, respectively.

Dependences of I_{sp} on the enthalpy of formation of the polynitrogen component are given.

Quantitative energy characteristics of compositions based on potentially available compounds containing carbon, oxygen or fluorine atoms in addition to high-enthalpy nitrogen. With a proper choice of a binder, such compositions easily reach the level $I_{sp} = 265$ sec. Some hypothetical compounds of this type can provide values of I_{sp} up to 290 sec.

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