Thermal decomposition of *cis*-2,4,6,8-tetranitro-1*H*,5*H*-2,4,6,8-tetraazabicyclo[3.3.0]octane

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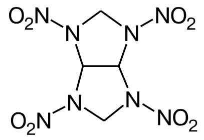
The thermal decomposition kinetics of *cis*-2,4,6,8-tetranitro-1*H*,5*H*-2,4,6,8-tetraazabicyclo[3.3.0]octane was measured in various solvents and in the solid phase by the manometric method. The general regularities for cyclic nitramines concerning the possibility of chain decomposition in hydrocarbon solvents, the kinetic display of cell effect in viscous media, a decrease in the decomposition rate in the solid state, and the quantitative description of this effect in terms of the model of monomolecular reactions in molecular crystals are supplemented and discussed. The dependence of the decomposition rate constants in solutions on the N—N bond lengths in a series of secondary nitramines was shown using the correct values of decomposition rate constants.

Key words: *cis*-2,4,6,8-tetranitro-1*H*,5*H*-2,4,6,8-tetraazabicyclo[3.3.0]octane, decomposition reaction, influence of medium, dependence of rate constant on N—N bond length.

Interest in studying the thermal decomposition of *cis*-2,4,6,8-tetranitro-1*H*,5*H*-2,4,6,8-tetraazabicyclo[3.3.0]-octane (**1**) is primarily caused by the intermediate position of this compound between monocyclic and framework nitramines, due to which it successfully supplements the series of secondary nitramines studied in detail (the data on their molecular structure and kinetics of decomposition in the solid phase and in various solvents are available) and makes this series more representative for establishing correlations between the structure and stability of the substance. The mentioned series of secondary nitramines includes seven compounds: dimethylnitramine (**2**), 1,3-dinitro-1,3-diazacyclopentane (**3**), 1,4-dinitro-1,4-diazahexane (**4**), 1,3,5-trinitro-1,3,5-triazacyclohexane (**5**), 1,3,5-trinitro-2-oxo-1,3,5-triazacyclohexane (**6**), 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (**7**), and 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo-[5.5.0.0^{5,9}.0^{3,11}]dodecane (**8**).



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Me_2NNO_2

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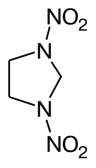

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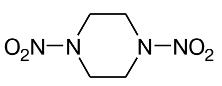

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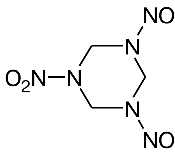

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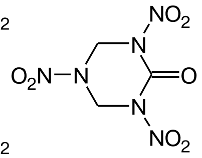

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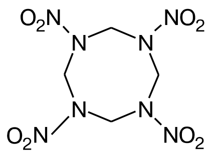

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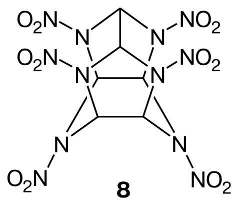

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The main data on the decomposition of secondary nitramines are given in the review.[1] The thermal stability differs by two orders of magnitude in the series of these compounds. The initial step of decomposition proceeds *via* the same mechanism: by the N—NO_2 bond cleavage. The pyramidal nitramine groups are considered to be more reactive. In these groups, the N—N bond elongates and its strength decreases because of the distortion of conjugation between the nitro group and trivalent nitrogen atom. However, an attempt to establish a relationship between the activation energy of decomposition and the length of the N—N bond in nitramines gave no certain results.[2] Unique regularities are observed for the decomposition of secondary nitramines in solutions. In chemically inert solvents, such as benzene, chlorobenzene, and dinitrobenzene, the decomposition rate decreases with an increase in the solvent viscosity due to the kinetic manifestation of the cell effect, while chain process begins to affect the decomposition reaction in alkyl-substituted aromatic and some other

Published in Russian in *Izvestiya Akademii Nauk. Seriya Khimicheskaya,* No. 6, pp. 1113—1118, June, 2011.

solvents with a decreased strength of the C—H bonds. The conditions for the appearance of chain reactions were formulated. Presently, it is of certain interest to predict the structures for decomposition of which these conditions are fulfilled. The decomposition of cyclic nitramines in the solid phase is considerably slower, as a rule, than that in the liquid phase, and these are the compounds that can most conveniently be used for experimental checking of the model of monomolecular reactions in the solid phase proposed earlier.[3]

Therefore, in this work, we studied the decomposition of nitramine **1** in various solvents and in the solid phase. The correlation between the decomposition rates and N—N bond lengths for cyclic nitramines was plotted using the correct data on these values.

Experimental

Nitramine **1** used in the work was purified by double recrystallization from acetone. The purity of the samples was monitored by the presence of an admixture region of gas evolution in the kinetic curves of decomposition of solid nitramine **1** at 140 °C. The decomposition kinetics was measured with a manometric setup provided for the pressure below 100 atm. The reactor was a glass ampule 0.5—5 mL in volume equipped with a falcate membrane with an arrow and placed in a metallic case with a window for the observation of deflections. The pressure was measured by the compensation method. This procedure makes it possible to carry out experiments at elevated temperatures almost in any solvents and to measure the decomposition kinetics at high degrees of filling the vessel with the substance (*m*/*V*).

Results and Discussion

Structure of nitramine 1. The crystal structure of nitramine **1** was described.[4] A molecule of **1** contains four nitramine groups differing by the N—N bond lengths and the structure of the pyramid of the amine nitrogen atom. In one of the nitramine groups, the N—N bond is strongly elongated and its length is 0.1414 nm. In this group, the angle between the plane C—N—C and the line of the N—N bond is maximum and equal to 41.1°, whereas for other groups the angles are 27.8°, 26.4°, and 19.1°. It is most likely that this is the group that is the most reactive in the decomposition of molecule **1**. There are no strong intramolecular spatial contacts involving the nitramine groups in structure **1**. The shortest distance (0.309 nm) is observed between the nitrogen atom of this nitramine group and the oxygen atom of the adjacent nitro group; however, even this distance does not exceed the sum of the van der Waals radii of atoms N and O (0.307 nm). It is most likely that the main reason for the strong elongation of the N—N bond is the shift of the nitro group, which violates its conjugation with the lone pair of the amine nitrogen, from the plane C—N—C.

Decomposition of nitramines in solutions. It is impossible to observe the decomposition of **1** in the liquid state, because it melts with decomposition at temperatures about 270 °C. It is difficult to measure the decomposition rate in vapors because of the low vapor pressure of the latter and, therefore, the single available possibility to determine the parameters of decomposition of molecules **1** in the free state is the study of this reaction in solution. When choosing solvents, we took into account the results of previous studies on the decomposition of nitramines in solution. It was found[5] for the decomposition of compound **5** that the reaction proceeds *via* the chain mechanism in solvents with a lowered strength of the C—H bond. This mechanism is proved by the retardation of the reaction upon the addition of inhibitors of chain processes and by the kinetic isotope effect of solvent. The chains appear due to the following: the aminyl and $^{\cdot}NO_2$ radicals formed at the first step of decomposition

$$>NNO_2 \rightleftharpoons >N^{\cdot} + {}^{\cdot}NO_2, \qquad (1), (-1)$$

transfer the free valence to the solvent RH to form the C-centered radical $R^{\cdot}$

$$>N^{\cdot} + RH \longrightarrow >NH + R^{\cdot}, \qquad (2)$$

$${}^{\cdot}NO_2 + RH \longrightarrow HNO_2 + R^{\cdot}. \qquad (3)$$

Then radical $R^{\cdot}$ reacts with the nitro group of nitramine transforming into the alkoxyl radical $RO^{\cdot}$

$${}^{\cdot}R + >NNO_2 \longrightarrow RO^{\cdot} + >NNO, \qquad (4)$$

and the latter generates radical $R^{\cdot}$ in the reaction of with the solvent

$$RO^{\cdot} + RH \longrightarrow ROH + R^{\cdot}. \qquad (5)$$

The decay of radicals $R^{\cdot}$ in the reaction with nitrogen monoxide NO, which is formed in large amounts upon decomposition, is slowed down, because NO exits to the gas phase and its concentration in the solution is low. The condition for chain growth is the absence of free radical traps, in particular, nitroso compounds, in the condensed products. This condition is fulfilled in the case of nitramine **5**. Since the rate of chain nucleation in reactions (2) and (3) increases with a decrease in the strength of the C—H bond, the dependence of the decomposition rate on the dissociation energy of the D_{C-H} bond is observed. The deuterium isotope effect of solvent appears in the same systems. The range of values of D_{C-H} in which the chain process occurs is 355—280 kJ mol^{-1}. At high values of D_{C-H}, reactions (2) and (3) do not occur, whereas at lower values reaction (4) ceases because of the low reactivity of radical $R^{\cdot}$. Outside this range of D_{C-H} the decomposition of nitramine **5** in solutions is monomolecular. One can compose the minimum set of solvents according to the published data,[5] and the occurrence of chain reactions can be judged by a change in the decomposition rates in these solvents. This set of solvents includes benzene, toluene, toluene-d$_3$, xylene, or another alkylated aromatic hydrocarbon. Similarly to compound **5**, nitramines **6** and **7** are prone[6] to chain decomposition. No chain reactions occur in the case of nitramines **2** and **8**, and the decomposition products of these compounds contain condensed inhibitors of chain reactions.

The examples for the kinetic curves of decomposition of nitramine **1** in various solvents are presented in Fig. 1. In spite of the low concentration (1 wt.%), the reactions proceed with acceleration. Experiments in solutions were carried out to the end. The final gas evolution depends weakly in the solvent and is about 6 moles per mole of substance at 180 °C. The rate constants of the initial noncatalytic stage of decomposition of nitramine **1** depend on the solvent (Table 1).

Table 1. Decomposition rate constants for nitramine **1** in solutions

Solvent	T/°C	k_{liq}/s^{-1}
Benzene	180	$2.6 \cdot 10^{-4}$
Toluene	180	$3.4 \cdot 10^{-4}$
Toluene-d$_3$	180	$2.3 \cdot 10^{-4}$
o-Xylene	180	$3.9 \cdot 10^{-4}$
1,5-Dimethylnaphthalene	180	$3.9 \cdot 10^{-4}$
o-Dichlorobenzene	180	$1.6 \cdot 10^{-4}$
Diphenyl	180	$1.5 \cdot 10^{-4}$
Benzene	170	$1.0 \cdot 10^{-4}$
Benzene	160	$3.6 \cdot 10^{-5}$
Benzene	150	$1.3 \cdot 10^{-5}$

The relative influence of the solvent on the decomposition rate of nitramines **1**, **2**, and **5—8** is shown in Table 2.

Table 2. Relative decomposition rate constants for secondary nitramines **1**, **2**, and **5—8** in solutions

Solvent	Compound					
	1	**2**	**5**	**6**	**7**	**8**
Diphenyl	0.50	0.79	0.38	0.86	0.37	0.60
o-Dichlorobenzene	0.50	—	—	0.50	—	—
Benzene	1.00	1.00	1.00	1.00	1.00	1.00
Toluene	1.30	0.79	1.28	1.80	1.71	0.88
Toluene-d$_3$	0.90	1.09	0.33	0.91	0.80	—
o-Xylene	1.50	0.75	3.37	—	3.37	0.9
1,5-Dimethylnaphthalene	1.50	—	—	1.61	—	—

Note. The decomposition rates of nitramines **6** and **8** were determined at 160 °C, those of nitramines **1** and **5** were determined at 180 °C, and the decomposition rates of nitramines **7** and **2** were determined at 200 °C and 230 °C, respectively. The data on nitramine **5** were published in Ref. 5, and those for nitramines **2** and **6—8** are in Ref. 7.

The data in Table 2 suggests that, in the case of nitramine **1**, in the solvents more viscous than benzene the decomposition rate is retarded, and the value of retardation is comparable with this effect for other nitramines. The general character of the phenomenon indicates that there is a common reason, possibly, the cell effect with the two- to threefold predomination of the recombination rate of $^{\bullet}NO_2$ and aminyl radicals over the decay rate of the latter due to the disproportionation with radical $^{\bullet}NO_2$ or intramolecular transformation. The increase in the decomposition rate of nitramine **1** in toluene, xylene, and 1,5-dimethylnaphthalene and the isotope effect of the solvent in toluene-d$_3$ indicate that properties of chain decomposition are manifested in the case of **1**. However, they are significantly less pronounced than those for compounds **5** and **7**. In this respect nitramine **1** is closest to compound **6**. In the case of nitramines **2** and **8**, chain reactions do not occur at all, which can be explained with allowance for the chain condition that requires the absence of free radical traps in the solution. It is known that the decomposition of nitramine **2** gives dimethylnitrosoamine, which is an efficient inhibitor of chain reactions, as one of the final products. The decomposition of nitramine **8** produces a large amount (15 wt.%) of condensed products containing double bonds C=C, C=N, and C=O and, perhaps, nitroso and nitro groups.[8] These compounds cannot be formed from nitramines **5** and **7**, which contain only methylene groups. The C—C bond in compound **1** can serve as a reason for the formation of stable nonvolatile compounds capable of playing the role of acceptors of free radicals and preventing the chain propagation in the solution.

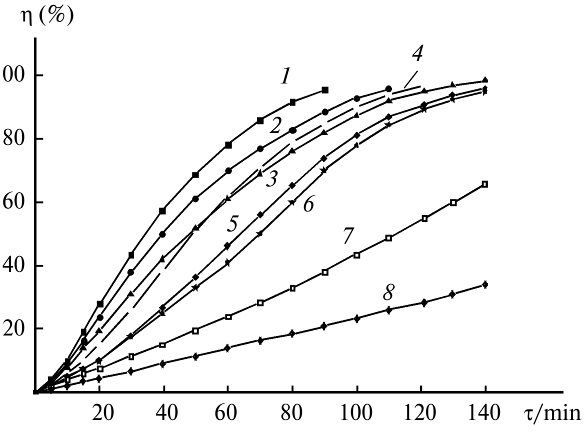

Fig. 1. Kinetic curves for the decomposition of nitramine **1** in *o*-xylene (*1*), toluene (*2*), benzene (*3*, *7*), toluene-d$_3$ (*4*), diphenyl (*5*), and *o*-dichlorobenzene (*6*, *8*) at 180 (*1—6*) and 170 °C (*7*, *8*).

The monomolecular decomposition of nitramine **1** in the inert solvent (benzene) is characterized by the activation energy $E_a = 159$ kJ mol^{-1} and preexponential factor $A = 10^{14.8}$ s^{-1}. The stability of nitramine **1** in solutions is lower than that of nitramines **7** and **5** and is close to that of compound **8**.

Decomposition of nitramines in the solid phase. The solid-phase decomposition of the closest analogs of **1**, compounds **7**, **5**, **6**, and **8**, occurs with considerable acceleration,[7—9] which is caused by the topochemical development of the process, autocatalysis by gaseous and condensed products, and the appearance of the liquid phase. In addition at low values of m/V and elevated temperatures, the reaction that occurs in the vapor phase makes the noticeable contribution to the decomposition rate of even such a low-volatile compound as **7**. The same regularities are observed in the case of nitramine **1** as well. The kinetic parameters for the decomposition of this substance in the solid state were determined in the temperature range 140—160 °C and at $m/V = 0.1$—0.3 g cm^{-1}. Under these conditions, the initial reaction rate is independent of m/V, because the role of the gas-phase decomposition is negligible, catalytic reactions proceed slowly at the early steps, and gas evolution is observed with a constant rate for rather long time. Upon the complete decomposition of 1 mole of solid **1** at 180 °C, 6.5 moles of gaseous products are evolved. Accepting that this value corresponds to the 100% conversion also at lower temperatures, the rate constant k_s for the initial non-catalytic stage of the reaction was calculated by the time of decomposition of nitramine **1** by 1%. At 140 and 160 °C the constant k_s is $6.7 \cdot 10^{-9}$ and $8.7 \cdot 10^{-8}$ s^{-1}, respectively. The kinetic parameters for k_s are the following: $E_a = 163.4$ kJ mol^{-1}, $A = 10^{12.87}$ s^{-1}.

Nitramine **1** is characterized by the strong retardation of the reaction in the solid phase. The retardation coefficient, which is determined as the ratio of rate constants in the liquid and solid phases $K_r = k_{liq}/k_s$, is equal to 260 for the reaction in benzene and 130 in *o*-dichlorobenzene that is closer to nitramine **1** by the molecular weight. The same high values of K_r are observed for some other cyclic nitramines. The available experimental values of K_r makes it possible to check the model of monomolecular reactions in the solid phase,[3,10] according to which the reaction in crystal occurs only in the sites of the strongly distorted, "fused" crystalline lattice, where the molecule gains rotational—vibrational mobility inherent in the liquid phase. In molecular crystals such conditions are most easily created on dislocations forming boundaries of microblocks. The fluctuation volume plays the role of defect in the volume of the undisturbed crystalline lattice. In the case of the volume reaction, formula (6) was obtained[3] for parameter K_r

$$RT\ln K_r = \Delta E = \Delta V^{\neq}{}_{add}{}^2/2\beta V_m, \quad (6)$$

where R is the universal gas constant, T is the absolute temperature, ΔE is the difference in the activation energies in the solid and liquid phases $E_s - E_{liq}$, β is the coefficient of isothermal compressibility, $V_m = M/\rho$ is the mole volume of the substance, and $\Delta V^{\neq}{}_{add}$ is the additional activation volume in the solid phase, which is considered as an increment of the cell volume occupied by the molecule to the sizes of the cavity in which intermolecular bonds are cleaved and the molecule gains the same free rotational—vibrational motion as in the liquid. In the expanded cell, the reaction occurs with the rate constant k_{liq} and the retardation effect of the solid phase is determined by the work ΔE consumed to elastic deformation of the cell. The simple and common for all molecules method for the estimation of the value of $\Delta V^{\neq}{}_{add}$ based on the relation of $\Delta V^{\neq}{}_{add}$ to V_m was proposed.[10] Thus, to calculate coefficient K_r by formula (6), one should know only the density and compressibility of the substance. The compressibility was calculated by the formula $\beta = 1/C_0{}^2\rho$, where C_0 is the sound velocity in crystal. In turn, C_0 was calculated by the Rao formula (see Ref. 11), which takes into account the chemical structure of the substance,

$$C_0{}^{1/3}M/\rho = \Sigma z_i B_i, \quad (7)$$

where z_i is the number of chemical bonds of this type, and B_i are increments of these bonds. The list of the known increments given in Ref. 11 makes it possible to apply Eq. (7) for the calculation of the value of C_0 and then parameter β for nitramines. The experimental and calculated values of K_r are presented in Table 3.

As can be seen from the data in Table 3, good correlation between the calculated and experimental data for K_r is observed, which confirms adequacy of the model. The closeness of the retardation effects found experimentally and calculated for the case of the homogeneous volume reaction indicates that no substantial decay occurs on defects of the crystalline lattice. According to the work,[13] the main defect in molecular crystals is presented by networks of dislocations forming boundaries of microblocks. In the most favorable for the reaction on defects case of $\Delta E = 0$, *i.e.*, in the assumption that no additional energy

Table 3. Experimental and calculated retardation coefficients K_r in the solid phase* for the decomposition of cyclic nitramines at various temperatures (T)

Compound	ρ /g cm^{-3}	T /°C	K_r	
			Experiment	Calculation
1	1.92	160	130	100
4	1.64	180	200[12]	300
5	1.84	160	300[12]	480
6	1.95	140	34[9]	56
7	1.78	260	90[7]	97
8	2.04	230	100[8]	144

* $K_r = k_{liq}/k_s$, the values of k_{liq} were taken from the data on decomposition of the corresponding nitramines in solutions in *m*-dinitrobenzene or *o*-dichlorobenzene.

expenses are required for the creation of "melted cell" on the surface and the reaction occurs with the same rate as in the liquid phase, the retardation coefficient K_r on the defects is inversely proportional to the fraction of molecules lying on the surface. For average sizes of molecules of 0.5—1.0 nm, the condition $K_r > 100$ is fulfilled at linear sizes of the microblock of 500—1000 nm. It is most likely that these sizes are typical of crystals of cyclic nitramines grown under the conditions of minor oversaturation.

Dependence of the rate constant of decomposition of secondary nitramines in solutions on the N—N bond length. In the series of secondary nitramines, which are compounds of one type by the character of electronic interaction in the group N—NO$_2$, the strength of the N—N bond should depend on its length (L_{N-N}) and, hence, the activation energy (E_a) of decomposition, which is the N—N bond dissociation, should correlate with L_{N-N}. However, the direct comparison of E_a with L_{N-N} is difficult because of the low accuracy of activation energy determination. The range of E_a changing in the series of the considered nitramines is 18 kJ mol^{-1} and the accuracy of measuring E_a rarely exceeds 8 kJ mol^{-1}. Therefore, it is more reasonable to use the decomposition rate constants determined at the same temperature as a measure of reactivity of nitramines. These constants change with the nitramine structure by two orders of magnitude and are determined with an accuracy of 10—15%. The decomposition rate of nitramines depends mainly on the value of E_a (preexponential factor (A) is almost constant[14]) and, hence, the reaction of decomposition of nitramines can be considered as an isoentropic series.

Since the literature data on the values of N—N bond lengths in the same compound diverge, the values of L_{N-N} were taken from the latest publications. The bonds with the maximum length were chosen for correlation. Polyfunctional molecules of nitramines usually contain one (compounds **1** and **6**) or two (compounds **3**—**5** and **7**, **8**) these bonds. For the correlation with L_{N-N} we chose the rate constant k_0, which represents the apparent rate constant for the decomposition of nitramine in benzene at 180 °C referred to one nitramine group with the longest N—N bond (Table 4). In the cases where at 180 °C the reaction was carried out not in benzene but in another solvent, the rate constant was recalculated by the value in benzene using the available data on the change in rate when the solvent is changed at temperatures close to 180 °C. The dependence $\log k_0$—L_{N-N} is shown in Fig. 2. It is seen that there is a relationship between these values. In spite of the scatter of values related to errors in estimation of k_0 and, possibly, to the influence of intermolecular interactions in crystal on L_{N-N}, the dependence presented in Fig. 2 can be used for the approximate estimation of constant k_0 of new compounds. It can be expected that nitramines with $L_{N-N} > 0.14$ nm would be close to nitramine **8** in stability and those with $L_{N-N} \approx 0.139$ nm would be close to compound **7**.

Table 4. Decomposition rate constants (k_0) for nitramines **1** and **3**—**8** in benzene at 180 °C and the maximum N—N bond lengths

Compound	k_0/s^{-1}	Reference	L^{max}_{N-N} /nm	Reference
1	$2.3 \cdot 10^{-4}$	This work	0.1414	4
3	$1.0 \cdot 10^{-4}$	15	0.1419	16
4	$2.5 \cdot 10^{-6}$	17	0.1373	18
5	$5.5 \cdot 10^{-5}$	7	0.1409	19
6	$1.1 \cdot 10^{-3}$	9	0.1438	20
7	$2.3 \cdot 10^{-6}$	7	0.1392	20
8	$5.5 \cdot 10^{-4}$	8	0.1446	21

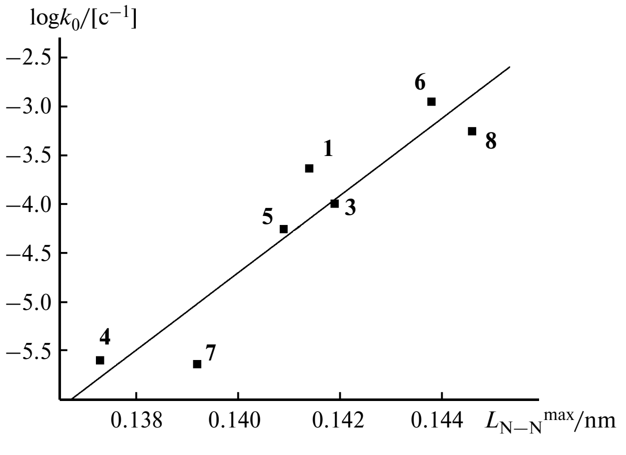

Fig. 2. Thermal decomposition rate constants (k_0) for nitramines **1** and **3**—**8** at 180 °C *vs* maximum N—N bond length (L^{max}_{N-N}).

This work was financially supported by the Russian Foundation for Basic Research (Project No. 10-03-91162-GFEN-a).

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Received March 4, 2011;
in revised form May 12, 2011