Alternative mechanisms of the primary act of gas-phase monomolecular thermal decomposition of N-methyl-N’-methoxydiazene-N-oxide according to the data of quantum chemical calculations

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Abstract. The mechanisms of the primary act of thermal decomposition of the simplest representative of the series of alkoxy-NNO-azoxy compounds – N-methyl-N’-methoxydiazene-N-oxide are studied using quantum-chemical density functional methods PBE, B3LYP, wB97XD with different sets of basic functions, as well as the composite G4 method. It is shown that the most probable channel of its thermal destruction, leading to the formation of experimentally observed reaction products, is isomerization because of rotation of the OCH3 group around the NO bond with the subsequent transfer of the CH3 group between oxygen atoms. In this case, the transfer of the CH3 group is the limiting reaction of the thermal decomposition of N-methyl-N’-methoxydiazene-N-oxide as a whole.

1. Introduction
Alkoxy-NNO-azoxy compounds (AZC) have the same elemental composition as secondary nitramines [1-3]. The latter are known to be widely used as explosives and components of solid rocket propellants [4-6]. Slightly inferior to nitramines in density, AZC, as a rule, surpass them in enthalpy of formation, thermal stability, and chemical stability. In addition, substituted alkoxy-NNO-azoxy compounds, such as cupferron ([Ph-N’(-O)=N-O]-NH4+), which releases nitric oxide under physiological conditions, are of interest as drugs, in particular, bioregulators of pressure [7, 8]. The first representatives of AZC (“Traube Salts”) were synthesized at the end of the 19th century [9]. Since the 1980s, when the first members of the homologous series of mono- and bis-alkoxy-NNO-azoxy compounds were synthesized, close attention has been paid to the study of AZC [10-26].

There are few works devoted to the study of the mechanism of thermal decomposition of these compounds despite the great practical interest in AZC [1, 22]. Considering that this issue is directly related to the safety of production, storage, and transportation, it is necessary, in our opinion, to pay more attention to this problem. When conducting the study, it was reasonable to start with the simplest representative of alkoxy-NNO-azoxy compounds – N-methyl-N’-methoxydiazene-N-oxide (1), which is an isomer of dimethylnitramine–(CH3)2N-NO2:
This communication is devoted to the quantum-chemical study of alternative mechanisms of the primary act of thermal decomposition of the specified compound.

The kinetics of thermal decomposition of compound 1 in the gas phase was studied in [1]. In particular, it was found that the process of thermal destruction of N-methyl-N’-methoxydiazene-N-oxide is homogeneous and corresponds to a first-order reaction, and the addition of NO does not inhibit decomposition, from which it was concluded that the process was not a chain one. The value of the activation energy ($E_a$), determined in the temperature range of 270-330°C, is equal to 204 ± 5 kJ/mol; log(A) 14.5±0.5 sec$^{-1}$ [1].

It is necessary to have an experimental value of the enthalpy of activation ($\Delta H^*$) for a correct comparison with the data obtained by us [27]. Using the formula for calculating the enthalpy $\Delta H^* = E_a - RT_{av}$, where $R$ is the universal gas constant, $T_{av}$ is the average temperature of the experiment. The value of the activation energy and the average temperature of the experiment (300°C) are taken from the work [1]. We get the value of $\Delta H^*$ equal to 199.2 kJ/mol.

The identification of thermal decomposition products in [1] was carried out on an LCH-8MD chromatograph. After analyzing the composition of the decomposition products, the authors assumed that the thermal decomposition of compound 1 proceeds according to the scheme shown in Figure 1. Moreover, the most probable primary act of thermal decomposition of N-methyl-N’-methoxydiazene-N-oxide, in their opinion, is the radical abstraction of the methoxyl radical.

In our opinion, there must be an alternative mechanism for the thermal decomposition of compound 1 [28], which can compete with the radical abstraction of the methoxyl radical. This assumption can be confirmed or refuted by quantum-chemical calculations, which were carried out in this work.

2. Calculation methods
A preliminary calculation of alternative mechanisms of the primary act and secondary processes of thermal destruction of N-methyl-N’-methoxydiazene-N-oxide was carried out by the PBE/L11 method in Priroda software package [29, 30] using the P-AUTOEXTREMUM shell to automate the iterative algorithm for studying the potential energy surface [31]. Calculation by this method in the specified program allows getting initial approximation for calculations of a higher level quickly but does not provide accuracy in quantitative estimates.

To refine the obtained Arrhenius parameters quantitatively in the study of the primary act of thermal decomposition of compound 1, we used the density functional methods [32, 33] B3LYP [34, 35] with a set of basis functions 6-31G (2df, p) [36, 37], wB97XD [38] with sets of basis functions 6-31G (2df, p) and Def2TZVP [39], as well as the composite method G4 [40].

It should be noted that although the description of secondary reactions [28] is not the purpose of this work, it is necessary at least in the minimum volume for the correct interpretation of the choice of...
the priority channel of primary reactions. Only one method B3LYP/6-31G (2df, p) was used to refine the PBE/L11 data obtained in the study of secondary reactions of the thermal decomposition of N-methyl-N'-methoxydiazene-N-oxide.

Calculations by the B3LYP, wB97XD and G4 methods were carried out using the Gaussian16 [41]. The calculation was carried out for the gas phase under normal conditions.

All found critical points on the potential energy surface were identified as minima or transition states by the absence or presence, respectively, of one negative eigenvalue of the matrix of second derivatives [41-46]. In turn, the correspondence of the found transition states to the investigated processes was established by means of descents along the reaction path from the saddle point to the reagents and products, and subsequent calculation (optimization) of the final structures of the descents [41-46]. In this case, the calculation was carried out for a singlet surface, and all solutions for localized points (minima and transition states) were checked for stability against perturbations imposed on the wave function [41, 43].

For most radical processes, it was assumed that the reverse processes of radical recombination proceed without activation, although this is not always the case [42]. In this case, the enthalpy of the reaction of radical abstractions was estimated from the difference between the sum of the enthalpies of formation of radicals and the enthalpy of formation of the initial compound:

$$\Delta H^\neq = (\Delta H_{R_1} + \Delta H_{R_2}) - \Delta H_{R_1-R_2}$$

However, it should be noted here that with such a calculation it is impossible to correctly estimate the rate constants of the reactions, since the structure of the transition state is unknown. Their values are highly overestimated [43].

In the case when the formation of hydrogen or other donor-acceptor bonds is possible during reactions of homolytic cleavage of bonds, the reactions of recombination of radicals, reverse to radical cleavage, are not activationless [42, 43]. The presence of a barrier to recombination is due to the formation of pre-reaction complexes at the initial stage. For a preliminary study of this kind of reactions, as a rule, at the initial stage, scanning techniques are used [41-43, 47], i.e., one of the geometric parameters, as a rule, in this case the length of the breaking bond, changes step by step, while the other geometric parameters are optimized relative to it. If a “break” is detected or a maximum is observed on the energy change curve depending on the scanned variable, then this point is taken as a starting point for direct search for the transition state [41-43]. In the case of finding the critical point of the potential energy surface, its correspondence to the transition state, as well as the subsequent correlation with the realized process, is carried out in a similar way for non-radical reactions, according to the procedure described above.

3. Results
We have considered the following alternative mechanisms of the primary act of N-methyl-N'-methoxydiazene-N-oxide (the corresponding numbers of the reaction products can be found in Table 1):

1. Rotation of the OCH$_3$ group around a bond NO:

$$\text{H}_2\text{N}^-\text{N}=\text{O}^-\text{N}^-\text{H}_2 \rightarrow \text{H}_2\text{N}^-\text{N}^-\text{O}^-\text{N}^-\text{H}_2 \quad (2)$$

$$\text{H}_2\text{N}^-\text{N}=\text{O}^-\text{N}^-\text{H}_2 \rightarrow \text{H}_2\text{N}^-\text{N}^-\text{O}^-\text{N}^-\text{H}_2 \quad (3)$$

These two processes differ only in the direction of rotation and, accordingly, the isomers that are mirror-like relative to each other.

2. Transfer of a CH$_3$ group between two nitrogen atoms:
The difference between these processes in the direction of deviation of the OCH$_3$ group relative to the plane of the molecule during the reaction.

3. Transfer of the CH$_3$ group between nitrogen and oxygen atoms:

4. Elimination of formaldehyde with simultaneous transfer of a hydrogen atom from the OCH$_3$ group to a nitrogen atom:

5. Formation of a cyclic intermediate through an oxygen bridge:

6. Radical cleavage of the N-O bond with elimination of the methoxyl radical:

7. Transfer of the CH$_3$ group between oxygen and nitrogen atoms:

8. Elimination of an oxygen atom:

Since the energy characteristics of this reaction were calculated as their difference between the data for the sum of the products and the reagent, we performed estimates for process (8) in two versions - the elimination of O in the singlet (process 11) and triplet (process 11’) states.

Table 1 shows the enthalpies of activation of reactions (2) - (11). All methods at a qualitative level give the same conclusions about the priority mechanism of the thermal destruction of the compound 1.
Table 1. Enthalpies of activation (kJ/mol) of alternative mechanisms of the primary act of gas-phase monomolecular thermal decomposition of N-methyl-N'-methoxydiazene-N-oxide (I).

| Process | Method          | PBE       | B3LYP    | wB97XD   | G4       |
|---------|----------------|-----------|----------|----------|----------|
|         | L11            | 6-31G(2df,p) | 6-31G(2df,p) | Def2TZVP |          |
| (2) 1 \rightarrow 2 | 17.7 | 15.8 | 14.0 | 17.1 | 15.9 |
| (3) 1 \rightarrow 2' | 17.7 | 15.8 | 14.0 | 17.1 | 15.9 |
| (4) 1 \rightarrow 3 | 203.4 | 224.7 | 237.0 | 245.2 | 233.9 |
| (5) 1 \rightarrow 3' | 203.4 | 224.7 | 237.0 | 245.2 | 233.9 |
| (6) 1 \rightarrow 4 | 270.2 | 288.9 | 302.5 | 362.6 | 290.1 |
| (7) 1 \rightarrow 5 | 231.2 | 282.6 | 309.8 | 369.1 | 279.6 |
| (8) 1 \rightarrow 6 | 225.4 | 235.9 | 296.3 | 307.7 | 258.5 |
| (9) 1 \rightarrow 7 | 236.8 | 221.4 | 238.2 | 227.5 | 255.3 |
| (10) 1 \rightarrow 8 | 271.8 | 297.8 | 311.6 | 310.8 | 327.4 |
| (11) 1 \rightarrow 9 | 395.8 | 562.4 | 565.9 | 614.3 | 484.3 |
| (11') 1 \rightarrow 9' | 326.0 | 291.3 | 295.5 | 330.7 | 286.9 |

As the Table 1 shows, the processes of radical abstraction of the oxygen atom have the highest enthalpies, regardless of the spin state (11) and (11'). This result was quite expected and did not come as a surprise. Also, high energy barriers are observed in the reactions of methyl group transfer between nitrogen and oxygen atoms (6) and (10), as well as the reaction of formaldehyde elimination (7).

A somewhat contradictory result in quantitative estimates was given by the quantum-chemical methods used by us on the process of formation of a cyclic intermediate (8), although there is still qualitative agreement, and it lies in the fact that the implementation of this process is unlikely.

According to our data, the most energetically favorable mechanisms of the primary act of thermal destruction of compound 1 are reactions of its isomerization because of rotation of the OCH\textsubscript{3} group around the NO (2) and (3) bond, which differ from each other, as mentioned above, only in the direction of rotation. The enthalpy of activation for these processes is very small, which indicates the almost free rotation of the above group, therefore, the reactions of further development of the process will play an important role here.

The processes of transfer of the CH\textsubscript{3} group between two nitrogen atoms (4) and (5), which differ from each other only in the arrangement in the transition state of the methyl group relative to the plane of the molecule, as well as the reaction of radical abstraction of the methoxyl radical (9), have rather close enthalpies of activation (Table 1). They are significantly lower than the barriers of other alternative processes (except for processes (2) and (3)). Based on the well-known fact [4, 42, 43] that the rate constants of radical processes are higher than molecular ones, then the probability of reaction (9) should be higher.

It should be noted that this result could well agree with the assumption made in [1] that the thermal decomposition of N-methyl-N'-methoxydiazene-N-oxide begins with the abstraction of the methoxyl radical. However, the barrier of reaction (9), calculated by us (Table 1), significantly exceeds the experimentally determined activation enthalpy of thermal destruction of N-methyl-N'-methoxydiazene-N-oxide 199.2 kJ/mol [1]. For density functional methods (Table 1), these differences are in the range of 22 - 38 kJ/mol.

The data of the composite method G4 for process (9) are somewhat out of the general picture. This method gives a significantly higher value of the barrier of the discussed reaction in comparison with the density functional methods and the experimental value. This result may be related to the fact that the G4 method [48], like many other composite methods [49], somewhat overestimates the enthalpies of free radical formation. And, since the barrier of the 7 \rightarrow 1 recombination reaction, inverse to the radical rupture (9), was estimated using formula (1), it becomes clear why the value of the G4 method is out of the general picture for the reaction under consideration. Although, as the Table 1 shows, even
this “dropout” of the value of the enthalpy of activation of the process (9), obtained by the G4 method, does not change the picture of competition between alternative mechanisms.

As we already noted in the introduction, the results of work [1] still do not exclude the implementation of alternative mechanisms, which means that the decisive role in the development of process (9), as well as in the case of reactions (2) and (3), will be played by secondary processes, as well as the conditions for the reaction of thermal destruction.

Figure 2. Scheme of isomerization of N-methyl-N'-methoxydiazene-N-oxide (1) according to the density functional method PBE/L11 and B3LYP/6-31G (2df, p) (in the diagram in parentheses). Relative enthalpies of formation of transition states (above-below arrows), reagents and products (below compounds) of reactions in kJ/mol. The enthalpy of formation of compound 1 is taken as zero. “Or” in the diagram means alternative paths that differ in the direction of rotation of the groups.

Figure 2 shows a scheme of all possible reactions of isomerization of N-methyl-N'-methoxydiazene-N-oxide. A closer look at Figure 2 shows that the transfer of the CH3 group between the oxygen atoms in compounds 2 and 2' with the formation of products 3 and 3' is much more favorable than the processes of the formation of the latter directly from compound 1. In other words, the more energetically favorable mechanisms of the primary reactions of thermal destruction of
compound 1 is the two-stage scheme isomerization $1 \rightarrow 2 \rightarrow 3$ or $1 \rightarrow 2' \rightarrow 3'$, compared to one-step reactions $1 \rightarrow 3$ or $1 \rightarrow 3'$.

The enthalpies of activation of processes $2 \rightarrow 3$ and $2 \rightarrow 3'$, obtained by B3LYP/6-31G (2df, p) method are equal to 183.9 kJ/mol, approximately 15 kJ/mol lower than the experimentally determined enthalpy of activation of thermal destruction of N-methyl-N'-methoxydiazene N-oxide 199.2 kJ/mol [1]. This deviation lies within the experimental error [43].

Further isomerization reactions of compound 3 have activation enthalpies (Figure 2) significantly lower than for reactions $2 \rightarrow 3$ or $2 \rightarrow 3'$, and, therefore, do not limit the process. Also, comparing the activation enthalpies of isomerization reactions $1 \rightarrow 2 \rightarrow 3$ or $1 \rightarrow 2' \rightarrow 3'$ with the enthalpy of reaction (9), it can be seen that the latter is less energetically favorable. According to the B3LYP/6-31G (2df, p) method, its barrier is almost 40 kJ/mol higher than that of reactions $2 \rightarrow 3$ or $2' \rightarrow 3'$. This result suggests that the abstraction of the methoxyl radical at the first stage can probably be realized only at sufficiently high temperatures and provided that the secondary processes of this radical abstraction will not limit the thermal destruction process.

It is also necessary to study the reactions of the further development of the process to confirm finally that the considered mechanisms of the primary act $1 \rightarrow 2 \rightarrow 3$ or $1 \rightarrow 2' \rightarrow 3'$ are priority.

The first reaction channel that we investigated is the abstraction of the NO radical from the isomer 3 and 3', since, as mentioned earlier, substituted alkoxy-NNO-azoxy compounds release nitric oxide under physiological conditions, demonstrating diverse bioregulatory activity [7, 8]. The reaction of NO detachment from intermediates 3 or 3', as shown in Figure 1 is not activationless. On the contrary, nitric oxide “clings” in every possible way to the atoms of the CH$_3$N$^\equiv$-O-CH$_3$ fragment. It should be noted here that the results of the PBE/L11 and B3LYP/6-31G (2df, p) methods gave slightly different geometric patterns of the evolution of the separation reactions. For PBE/L11, we found mirror isomers with an N-N bond length of 168.3 pm (in Figure 1, structures 10 and 10'). It is from these structures that further separation of NO occurs (reactions $10 \rightarrow 13 \rightarrow 14$ and $10' \rightarrow 13' \rightarrow 14'$). We failed to localize structures 10 and 10' by the B3LYP/6-31G (2df, p) method, and the abstraction of nitric oxide occurs from structures 9 and 9' with an NN bond length of 136.6 pm (reactions $9 \rightarrow 15 \rightarrow 16 \rightarrow 17$ and $9' \rightarrow 15' \rightarrow 16' \rightarrow 17'$). Nevertheless, despite the described differences, both methods allow us to conclude that the abstraction of NO from the isomers of N-methyl-N'-methoxydiazene-N-oxide with structures 3 or 3' does not proceed without activation. On the path of the discussed reactions, transition states are localized.

With further stretching of the N-N bond in structures 14 and 14' (PBE/L11) or 17 and 17' (B3LYP/6-31G(2df, p)), technical difficulties arose due to sufficiently large distances and very small differences in energies. Therefore, we estimated the relative barrier of the final detachment of nitric oxide from the difference in the sums of the enthalpies of formation of radicals CH$_3$N$^\equiv$-O-CH$_3$ and NO$^*$ (18) and compounds 1 according to formula (1). The obtained estimates of 143.1 kJ/mol (PBE/L11) and 111.4 kJ/mol (B3LYP/6-31G(2df, p)) are close to the relative barriers of reactions $13 \rightarrow 14$ or $13' \rightarrow 14'$ and $16 \rightarrow 17$ or $16' \rightarrow 17'$ respectively. Therefore, we believe that further detachment of nitric oxide occurs with a high degree of probability without activation and does not limit the entire process.

Alternative to NO$^*$ elimination channel for thermal decomposition of N-methyl-N'-methoxydiazene-N-oxide associated with the elimination of formaldehyde from 3 or 3':

was investigated by us earlier by the density functional methods PBE and B3LYP/6-31G (2df, p) [28]. This channel leads to the formation of reaction products such as CH$_2$O, N$_2$O, CH$_4$, N$_2$, CO, CO$_2$,.
CH₃OH, etc. those products that are observed in the experimental study of the thermal gas-phase decomposition of N-methyl-N’-methoxydiazene-N-oxide [1]. The reactions studied by us have significantly lower barriers than the limiting stages 2 \rightarrow 3 or 2’ \rightarrow 3’.

4. Conclusions

Thus, during the thermal decomposition of N-methyl-N’-methoxydiazene-N-oxide, the most probable mechanism of the primary act leading to the formation of experimentally observed reaction products [1] is the rotation of the OCH₃ group around the NO bond with the subsequent transfer of the CH₃ group between oxygen atoms. In this case, rotation has a very small activation barrier, i.e. is practically free, and the transfer of the methyl group limits the process of thermal destruction of the compound under study.

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