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# QUASI-EQUILIBRIUM PROCESSES OF ELECTRONIC EXCITATION RELAXATION IN THE 1.5-DIAZIDOPYRIMIDINE MOLECULE

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***Abstract***—*This work reports combined experimental and theoretical investigations of quasi-equilibrium relaxation of electronic excitation in 1.5-diazidopyrimidine (1.5-DAP) and discusses its practical relevance. Analysis of the energy structure of the molecule shows that the first two singlet excited states* ($S_1$ *and* $S_2$) *arise from quantum transitions to dissociative* $\pi\sigma^*$ *states: S1 is associated with excitation localized on the azido group at position 5, whereas* $S_2$ *is localized on the azido group at position 1; the corresponding wave functions are spatially separated. The next two singlet states correspond to quantum transitions to* $\pi\pi^*$*-states that form the absorption spectrum of the molecule. The relaxation of electronic excitation of the molecule is described in terms of a quasi-equilibrium pathway that enables localization of excitation at higher energy levels. Because there is an energy barrier in* $S_1$ *prevents N–N bond cleavage along this channel, the process of excitation relaxation proceeds to* $T_3(\pi\pi^*)$ *and subsequently to* $T_2(\pi\sigma^*)$*, which corresponds to excitation localized on the azido group at position 5. Consequently, the molecule dissociation occurs only via the single dissociative state* $T_2(\pi\sigma^*)$*. Relaxation of excitation from* $T_2$ *to the lowest triplet excited state* $T_1(\pi\pi^*)$ *is found to be forbidden, which provides a high quantum yield of azido-group photodissociation. It is shown that all other channels of electronic excitation relaxation led to the relaxation of the molecule to the* $T_2$ *state, i.e. the process is quasi-equilibrium. The consequence of such localization is the dissociation of the molecule with the release of a nitrogen molecule and nitrene. Nitrene, being a highly reactive particle, is widely used in molecular and nanoelectronics to create photoresists, as well as intermediates in nanotechnology.*

**Keywords**—Quasi-equilibrium relaxation of electronic excitation in a molecule, dissociative states of a molecule, configurational interaction, molecular photodissociation mechanism, use of azides.

## I. INTRODUCTION

Many molecular compounds are used in nanoelectronics technology, for the functionalization of nanotubes and nanofibers [1] – [4], for the needs of moletronic, etc. [8], [9]. It is important in this regard that molecular elements can provide the creation of computational elements, having small sizes. Therefore, they can provide further minimization of computing elements. Azides, being able to create highly reactive intermediate products under the action of light, have been widely used in molecular and nanoelectronics as photoresists or intermediate products in nanotechnology [11]. On the other hand, the study of electronic excitation relaxation processes in molecules with a Xe-O bond allows solving a number of fundamental problems associated with non-equilibrium and quasi-equilibrium electronic excitation relaxation processes. In addition, molecules with a Xe-O bond have unique properties that allow them to be used for various practical needs. It is known [1] that the substance Xe-O has the ability to explode when a single electron enters it. Diazonium salts and azides have the same property, although to a much lesser extent. Therefore, they exhibit a high photochemical property from a highly excited state. The same property, but with a much lower quantum yield, is also exhibited by dye molecules [1] – [4], as a result of which they fade under UV irradiation. However, to date, few scientific studies have been devoted to the study of this problem.

## II. PROBLEM STATEMENT

The behavior of molecules in highly excited states, non-equilibrium and quasi-equilibrium relaxation of electronic excitation of molecules and

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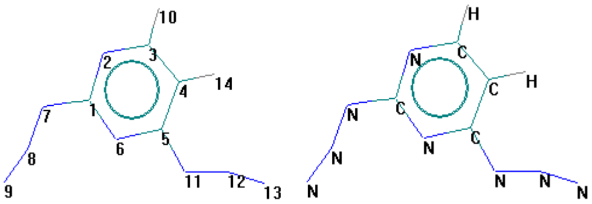
photodissociation of molecules are urgent fundamental problems of modern physics. The problem is that according to the laws of photochemistry, electrons from highly excited states relax in a non-equilibrium manner to the lowest excited triplet state, in which photochemical processes are possible [1]. Our studies show that photochemical processes occur mostly from the highly excited state, which indicates quasi-equilibrium relaxation of excitation [1] – [4]. The use of molecular structures for various technical problems, in particular, for molecular and nanoelectronics, requires the manufacture and study of the properties of these structures [5] – [7]. Such studies contribute to filling the database from which it is possible to select those structures that best meet the needs of moletronics and nanotechnology. In this regard, azides, which are characterized by intense absorption spectra in the near ultraviolet region and high quantum yields of photodissociation of these molecules, look promising [8], [9]. The important properties of this class of azides have led to their widespread use also in pharmaceutical science and practice [10]. In this regard, this article is devoted to research aimed at solving the problem of quasi-equilibrium relaxation of electronic excitation and mechanisms of photodissociation of pyrimidine diazide.

## III. RESEARCH METHODS

In our work, we studied the energy structure and processes of quasi-equilibrium relaxation of electronic excitation in 1,5-DAP molecules, which are accompanied by dissociation of the 1,5-DAP molecule from the excited state:



1,5-DAP molecule

Therefore, we studied the possibility of dissociation of the bond between atoms 7 and 8, as well as between atoms 11 and 12 in the 1,5-DAP molecule. In addition, we studied the relaxation processes that affect this possibility.

Experimental studies were carried out in liquid (hexane, ethanol) and solid polymer solutions at room temperature. The absorption spectrum of 1,5-DAP solutions contains broad intense bands with a maximum at 240 nm and 285 nm, as well as weak bands in the region of 320 nm and 341 nm. The molecules were excited by monochromatic radiation of a mercury lamp ($\lambda$ = 313 nm). The absorption spectra, as well as the change in optical density during the dissociation of the studied molecule, were recorded using a Specord 210 spectrophotometer. The quantum yield of photodissociation of the studied molecule was found by comparison with the quantum yield of a known solution (potassium ferrioxalate) [1]. Theoretical studies of the energy structure of the 1,5-DAP molecule were carried out using the semi-empirical quantum-mechanical calculation method MNDO [12], which included the configurational interaction between 12 occupied and 12 unoccupied molecular orbitals (MOs). At the same time, the occupied electrons were 29 MO.

## IV. RESULTS OF THE RESEARCH CONDUCTED

The calculations indicate that the singlet and triplet excited states are of $\pi\pi^*$ and $\pi\sigma^*$ type (Table I). Importantly, the two lower excited singlet states correspond to $\pi\to\sigma^*$ quantum transitions and are characterized by small extinction coefficient. Excitation of a molecule in the third (S3), fourth (S4) and higher $\pi\pi^*$ singlet states shape the absorption spectrum of the molecule.

To characterize the magnitude of the extinction coefficient for a quantum transition from level $m$ to level $n$, the oscillator strength $f$ [1] is introduced; its values for different quantum transitions are given in Table I.

$$f_{mn} = \frac{2m\omega_{mn}\,|D_{mn}|^2}{e^2\hbar}, \qquad (1)$$

where $D_{mn}$ is the matrix element of the vector of the electric dipole moment of the quantum transition $m\to n$, which is found by the formula:

$$D_{mn} = -e\int \psi_m^*(r,t)\,r\,\psi_n(r,t)\,dv. \qquad (2)$$

Quantum transition probability can be expressed as:

$$p_{mn} = \frac{4\pi^2}{\hbar^2}\,|\vec{I}\vec{D}_{mn}|^2\,\rho(\omega_{mn}). \qquad (3)$$

Here $\vec{I}$ is the ort lying in the plane of polarization of the electromagnetic wave, $\rho(\omega_{mn})$ is the energy density of the electromagnetic wave.

Applying formulas (1) – (3) to quantum transitions in $\pi\pi^*$ and $\pi\sigma^*$ states, we note that all quantum transitions to singlet states are symmetry-allowed. In this case, the dipole moments of quantum transitions in $\pi\pi^*$ states are polarized in the plane of the molecule, and in $\pi\sigma^*$ states – perpendicular to the plane. The difference in the magnitude of the oscillator strength is caused only by the spatial prohibition, i.e., the wave-function overlap integral for excitation into $\pi\sigma^*$ states is close to zero, while no such prohibition when the molecule is excited in the $\pi\pi^*$ state.

TABLE I. QUANTUM TRANSITIONS IN THE 1.5-DAP MOLECULE

| **Multiplicity, symmetry** | **Attribution (MO numbers)** | **λ, nm** | ***h*ν, eV** | **Oscillator strength, *f*** |
|---|---|---|---|---|
| $T_1$ π→π* | 29→30 | 613 | 2.023 | 0 |
| $T_2$ π→σ5* | 28, 29→31 | 543.7 | 2.280 | 0 |
| $T_3$ π→π* | 28→30,<br>29→32 | 513.1 | 2.416 | 0 |
| $T_4$ π→σ1* | 28, 29→33 | 484.2 | 2.561 | 0 |
| $S_1$ π→σ5* | 28, 29→31 | 476.2 | 2.604 | 0.0001 |
| $T_5$ π→π* | 29→35 | 455.3 | 2.723 | 0 |
| $S_2$ π→σ1* | 28, 29→33 | 432.4 | 2.867 | 0.0001 |
| $T_6$ π→π* | 29→32, 34 | 432.1 | 2.869 | 0 |
| $T_7$ π→σ5* | 28, 29→36 | 370.5 | 3.346 | 0 |
| $T_8$ π→σ1* | 28, 29→37 | 365.9 | 3.389 | 0 |
| $T_9$ π→π* | 28→32 | 350.9 | 3.533 | 0 |
| $T_{10}$ σ→π* | 27→30,<br>32, 34 | 348.5 | 3.558 | 0 |
| $S_3$ π→π* | 29→30 | 346.8 | 3.575 | 0.1382 |
| $S_4$ π→π* | 29→32 | 333.1 | 3.722 | 0.2327 |
| $S_5$ π→σ5* | 28, 29→36 | 316.7 | 3.915 | 0.0088 |
| $S_6$ π→σ5* | 28→30,<br>29→34 | 316.4 | 3.919 | 0.1020 |

It has been shown in Refs. [1], [3] that the processes of dissociation of a molecule into fragments are possible exclusively from $\pi\sigma^*$- states. Therefore, it should be expected that in the presence of relaxation of excitation to triplet $\pi\sigma^*$- states we will be able to see the dissociation of the molecule. Therefore, one of the states $T_2$ and $T_4$ will oversee the dissociation of the azido group upon excitation of the molecule. The dependence of the energies of excited states upon dissociation of the molecule was analyzed starting from the quasi-equilibrium state $T_4(\pi\sigma^*)$, where the σ*-MO is localized on the azido group at position 1 (Fig. 1), and then from the state $T_2(\pi\sigma^*)$, where the σ*-MO is localized on the azido group at position 5.

Upon elongation of the N–N bond, the $T_4$ state intersects lower triplet states, becoming the $T_2$ state, and finally intersects the $T_1(\pi\pi^*)$ state. Because the $\pi\sigma^*$- and $\pi\pi^*$-states are of different nature (Table I), relaxation from $T_2$ to $T_1$ was turned out to be forbidden. This, in turn, provides a high quantum yield of the photodissociation of the azido group with the formation of molecular nitrogen and nitrene. The quantum yield reaches 1.0 in solutions (in ethanol 2.0) and is 0.8 in a solid polymer matrix. The decrease in the quantum yield of the photodissociation of the molecule in a solid polymer matrix is associated with steric hindrance, which promotes the process of relaxation of the excitation to the $T_1$ state.

The study of the absorption spectra of 1.5-DAP molecules showed that solutions of these compounds have a broad absorption band in the region λ = 313 nm. Therefore, the excitation of the 1.5-DAP molecule states that it provides the appearance of an absorption band in the region λ = 313 nm occurs in the singlet states $S_3$ and $S_4$. From these states, the molecule relaxes at a high speed to the states $S_2$ and $S_1$, which are dissociative (Fig. 1).

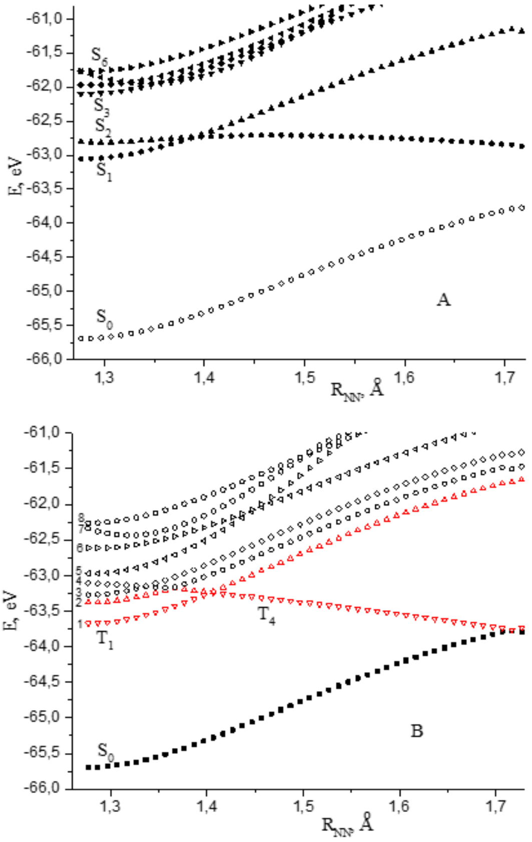
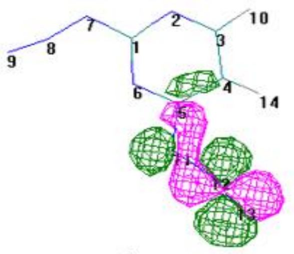
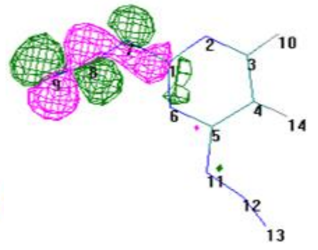


Fig. 1. Energy structure of the 1.5-DAP molecule depending on the length of the dissociating bond in the azido group at position 1 of the molecule for singlet (A) and triplet (B) excited state

To describe the processes of relaxation of electronic excitation from $\pi\sigma^*$-states, it is necessary to pay attention to the structure of the corresponding σ*-MOs at equilibrium distances between atoms:



σ*-MO-31



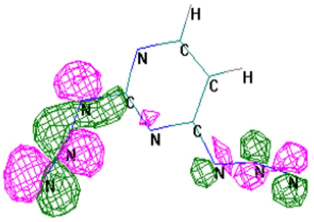
σ*-MO-33

As can be seen from the above MO structures, these MOs are spatially separated. Therefore, it could be assumed that the spatial prohibition of relaxation of electronic excitation between the singlet $S_2$ and $S_1$ states, as well as between the $T_4$ and $T_2$ states, would contribute to the dissociation of not only the azido group in position 5, but also the azido group in position 1.

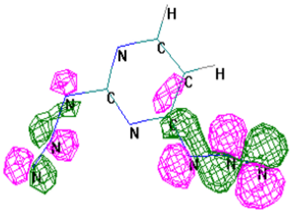
Let's see how the processes of relaxation of electronic excitation develop when it is localized in the $S_2$ or $T_4$ states.

For a molecule in the ground-state geometry, the electronic relaxation $S_2 \rightarrow S_1$ is strongly slowed down. Dynamic processes in the molecule will cause the elongation of the bond between atoms $N_7$ and $N_8$ (Fig. 1), causing the energy surfaces of the states $S_2$ and $S_1$, as well as $T_4$ and $T_2$, intersect. This fact enhances configuration interaction and modifies the MO shapes for the corresponding σ*-states.

When the $N_7$–$N_8$ bond in the 1–$N_3$ group is elongated to 1.387 Å (the intersection point of two energy surfaces of σ* states), the σ* MOs have the form:



σ*-MO-31



σ*-MO-33

As a result of the transformation of the shape of the corresponding σ*-MOs, the interaction between the states appears. In the region of intersection of the energy surfaces of these states, the interaction between the states caused the splitting of the configuration surface. The splitting value for the singlet states $S_2$ and $S_1$ is 0.0085 eV.

The triplet states $T_4$ and $T_3$ intersected with almost no splitting at a bond length of 1.337 Å, such that the $T_4$(πσ*) state becomes $T_3$(πσ*) state. Upon further bond elongation, the $T_3$(πσ*) state intersects $T_2$ (πσ*) state at 1.367 Å and becomes $T_2$(πσ*) state localized on group 1 with a splitting of 0.02 eV. Finally, the $T_2$(πσ*) state intersects with the $T_1$(ππ*) state. In this case, no splitting of the energy surfaces is observed due to the spatial prohibition.

Note that $kT$ at room temperature is 0.045 eV. This fact causes an instantaneous non-equilibrium relaxation of the electronic excitation between the two (πσ*)-states on the way to their intersection. As a result, further elongation of the $N_7$–$N_8$ bond toward the $T_2$(πσ*) – $T_1$(ππ*) intersection does not proceed, and the dissociation of the 1–$N_3$ group turned out to be impossible.

Singlet–triplet conversion can be explained in terms of additional mixing of singlet and triplet states due to perturbation – spin-orbit interaction, i.e., by interaction between the orbital and spin magnetic moments of electrons.

The spin-orbit interaction operator can be written as

$$H_{SO} = \zeta[LS], \tag{4}$$

where ζ is a parameter depending on the potential field of the nuclei (heavy atom effect). For hydrogen-

like atoms $\zeta = \dfrac{Ze^2}{2m^2c^2r^3}$.

This interaction leads to wave-function mixing, such that the triplet state wave function can be represented as:

$$\psi_T^{SO^\circ} = \psi_T^{0^\circ} + {}^\circ\lambda\psi_S^0, \tag{5}$$

where

$$\lambda^\circ = \left| \frac{\int \psi_S^0 \hat{H}_{SO} \psi_T^0 d\tau}{E_T{}^\circ - {}^\circ E_S} \right|. \tag{6}$$

In fact, to find the parameter of mixing singlet states to the selected triplet state, it is necessary to calculate the value of λ for all singlet MOs and then find which of these MOs makes the main contribution to the mixing. The value of λ will determine the value of the dipole moment of the quantum transition:

$$D_{S_0 \rightarrow T_1}{}^\circ = {}^\circ\int \psi_S^0 e\vec{r}\psi_T^{SO} dv^\circ = {}^\circ\lambda D_{S_0 \rightarrow S}. \tag{7}$$

Here, an important condition for the manifestation of the $S_0 \rightarrow T_1$ transition is the inequality of the magnitude of the dipole moment of the quantum transition $D_{S_0 \rightarrow S}{}^\circ \neq {}^\circ 0$, that is, the mixing of the triplet state must occur with such a singlet state that there is no symmetry or overlap prohibition.

As follows from formula (6), the value of λ will be the greater, the smaller the difference $E_S - E_T$ between the energies of the states whose MOs are mixed. In addition, λ ~ ζ, therefore, is found by the field of the nuclei, or the probability of finding MOs near atomic nuclei [1].

As a result, the molecule relaxes into the dissociative state $T_2$(πσ*), localized at the azido group at position 5.

Based on the above, it is clear that the nonradiative relaxation channel of electronic excitation in isolated 1.5-DAP molecules or in liquid solutions into the $T_1$ state is insignificant, which ensures a high quantum yield of photodissociation of the molecule upon excitation into singlet ππ*-states.

Upon further elongation of the N–N bond to 1.75 Å, the energy surface of the $T_2$ state (πσ*) intersects with the $S_0$ ground state. Therefore, Therefore, N–N bond dissociation yields a product with a ground triplet state. Thus, nitrene is formed – a molecule with a single C–N bond and two non-bonding MOs localized on the nitrogen atom. These two electronic orbitals make nitrene a highly reactive particle that provides crosslinking of solid solvent molecules, i.e., it is a promising intermediate for phototechnology processes of various purposes, including molecular and nanoelectronics [13], [14].

## V. CONCLUSIONS

Based on experimental and theoretical studies of the photodissociation of the azido group in position 1 of the 1.5-DAP molecule, the following is shown.

*1)* The first two singlet states of 1.5-DAP molecule are due to quantum transitions to dissociative πσ* states, the first is localized on the azido group at position 5, whereas the second is localized at position 1 implying spatial separation of the corresponding wave functions. The next two singlet states correspond to quantum transitions to ππ* states, which form the absorption spectrum of the molecule.

*2)* The $S_2$(πσ*) state is dissociative: upon elongation of the N–N bond in the 1–$N_3$ group, the system energy decreases toward S1, while the wave functions transform and overlap, enabling non-equilibrium relaxation into S1 state.

*3)* In the $S_1$(πσ*) state, a barrier of 0.218 eV prevents N–N bond cleavage, thereby excluding this dissociation channel. The process of excitation relaxation continues to $T_3$(ππ*) state, and then to $T_2$(πσ*) state, localized on the azido group in position 5 of the molecule, thus, $T_2$(πσ*) is the only dissociative state in the proposed scheme

*4)* Upon molecule excitation into $S_3$ or $S_4$ state, relaxation of the molecule can proceed to $T_8$(πσ*) state and then to the dissociative $T_4$(πσ*) state. However, along the N-N-bond elongation, relaxation to $T_2$(πσ*) state occurs, leaving it as the only dissociation channel.

*5)* The dissociative state formed via quasi-equilibrium relaxation of the electronic excitation of the molecule produces nitrene, a highly reactive molecule, widely used in phototechnological processes.

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**П. О. Кондратенко, А. П. Поліщук, Т. М. Сакун, Г. Є. Марінченко, І. О. Бородій. Квазірівноважні процеси релаксації електронного збудження в молекулі 1,5-діазидопіримідину**

Роботу присвячено вивченню на підставі експериментальних і теоретичних досліджень процесів квазірівноважної релаксації електронного збудження молекули 1,5-діазидопірімідину (1,5-ДАП) та її практичного використання. При вивченні енергетичної структури молекули показано, що перші два синглетні стани молекули ($S_1$ і $S_2$) зумовлені квантовими переходами в дисоціативні πσ*-стани, перший з яких відповідає локалізації на азидогрупі в положенні 5, а другий – в положенні 1. Хвильові функції відповідних станів просторово відділені. Наступні два синглетні стани відповідають квантовим переходам в ππ*-стани, які формують спектр поглинання молекули. Показано, що релаксація електронного збудження молекули описується квазірівноважним процесом, який дозволяє локалізації збудження на вищих енергетичних рівнях. Оскільки в стані $S_1$ на шляху до розриву N–N-зв'язку існує енергетичний бар'єр, який виключає цей канал дисоціації, продовжується процес релаксації збудження до стану $T_3$(ππ*), а потім до стану $T_2$(πs*), який відповідає локалізації збудження на азидогрупі в положенні 5 молекули. Як наслідок, в реалізується дисоціація молекули лише через єдиний дисоціативний стан $T_2$(πσ*). Релаксація збудження зі стану $T_2$ до нижнього збудженого стану $T_1$(ππ*) виявилась забороненою, що забезпечує високий квантовий вихід фотодисоціації азидогрупи. Показано, що всі інші канали релаксації електронного збудження приводять до релаксації молекули в стан $T_2$, тобто процес є квазірівноважним. Наслідком такої локалізації є дисоціація молекули з виділенням молекули азоту і нітрена. Нітрен, будучи високореакційною, частинкою, широко використовується в молекулярній і наноелектроніці для створення фоторезистів, а також як проміжних продуктів в нанотехнології.

**Ключові слова**: квазірівноважна релаксація електронного збудження в молекулі, дисоціативні стани молекули, конфігураційна взаємодія, механізм фотодисоціації молекули, використання азидів.

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