

Interaction of nitrobenzene by ArF-laser

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A single-frequency process of interaction between the radiation of an excimer ArF laser and the vapor phase of nitrobenzene is considered. The fluorescence of vibrationally excited nitric oxide molecules formed during a photofragmentation of nitrobenzene is investigated. The influence of inert gases He, Ne and N₂ on the fluorescence of the excited states of NO C²Π and NO A²Σ, D²Σ has been demonstrated. In a nitrogen environment, the fluorescence of NO A²Σ (ν' = 0) is enhanced due to the intermolecular non-radiative energy transfer from the metastable level N² A³Σ to the electronic level of NO A²Σ.

Keywords: nitro compound, photofragmentation, nitric oxide, fluorescence.

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Introduction

When studying the processes of photodissociation of complex organic compounds, measuring the lifetime of excited states of molecules, and the quantitative ratio of reaction products, several laser sources are generally used in well-known experimental methods „pump-probe“. This method has some similarity with the optical method of substance investigation through photo-fragmentation of the main molecule followed by laser-induced fluorescence of its characteristic fragments (FF-LIF) [1]. The process of laser interaction with the substance can occur at one or multiple wavelengths of the radiation. In two-frequency interactions, special attention is paid to the effective choice of the fragmenting and subsequent resonantly exciting laser source based on the maximum absorption cross-section. In the case of the single-frequency FF-LIF method, several conditions are met: the studied molecules have a sufficiently high absorption cross-section for the used wavelength of radiation, absorption leads to photodissociation of the molecule, the formed simple photo-fragments are suitable for the subsequent laser-induced process, and the radiation pulse duration is sufficient for the duration of all sequential processes. If the energy gaps between the ground and excited states of molecules are large, multiphoton interaction processes using ultra-short duration laser pulses are employed [2–5].

Detection by fluorescence of vibrationally excited fragments of nitrogen oxides from organic and inorganic nitro compounds R-NO_x is a relevant scientific research task. Since substances of this class are formed and pollute the lower atmospheric layer mainly from anthropogenic sources: metallurgy during high-temperature combustion of fossil fuels, automobile emissions, thermal power plants, as

well as a by-product of the chemical nitric acid industry. Special significance in the safety research area is given to studies on remote detection of fluorescence of nitrogen oxide fragments obtained from nitro-containing high-energy materials (HEM) under laser exposure [6–9]. Fluorescence of vibrationally excited fragments of nitrogen oxide is also of interest in studying chemiluminescent reactions NO_x, occurring in the upper atmosphere as a result of solar radiation photolysis [10].

Effective absorption of most nitro-containing substances is located in the far ultraviolet spectral range (UV-C) [11]. The organic compound nitrobenzene C₆H₅NO₂ has the simplest electronic structure among aromatic nitro compounds and serves as a useful model for studying the dynamics of photochemical reactions of nitro-containing substances.

Electronically excited singlet states of aromatic nitro compounds are often considered practically non-fluorescent. Nitrobenzene (NB) does not exhibit bright emission capability at room temperature because its spectral transitions are spaced far apart. Deactivation of the fluorescent state is explained by the rapid intersystem crossing of the singlet-triplet transition $S_{n\pi^*} \rightarrow T_{\pi\pi^*}$ occurring on a nanosecond timescale. Rapid or ultrafast nonradiative conversion of excited singlet states of aromatic nitro compounds indicates common features of their structure, where the nitro group NO₂ shows strong electron-acceptor properties, causing a reduction of fluorescence quantum yield. Only weak phosphorescence of nitrobenzene is known to be possible in optical interactions at cryogenic temperature 77 K [12].

Due to the difficulty of obtaining fluorescence from aromatic nitro compounds, the optical FF-LIF method allows indirect determination of the initial substance by narrowband fluorescence of main characteristic fragments after photo-fragmentation. The present work presents

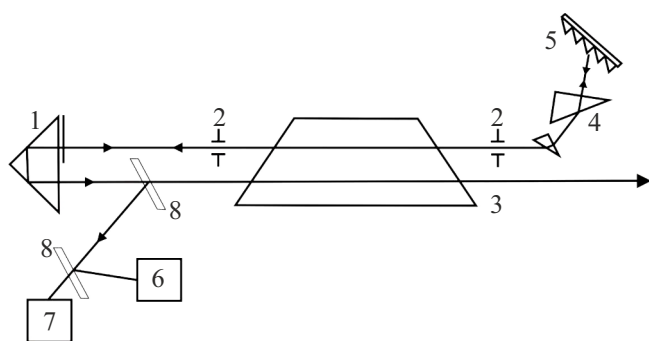


Figure 1. Optical scheme of the laser: 1 — rectangular prism with reflectivity coefficient 10%, 2 — diaphragm 6×3 mm, 3 — active medium, 4 — prismatic telescope, 5 — diffraction grating 2400 Grooves/mm, 6 — profilometer SP620U, 7 — wavelength meter WS6, 8 — beam splitter plate.

Table 1. ArF Laser Parameters

Parameter	Value
Central wavelength, nm	193.3
Tuning range, nm	193.05-193.7
Pulse duration (FWHM), ns	10
Line width, pm	20
Maximum energy, mJ	10 (narrowband) or up to 200 (broadband)
Repetition frequency, Hz	20
Divergence, mrad	< 0.8
Beam dimensions $a \times b$ mm	5×10

results of studying temporal and spectral characteristics of fluorescence of vibrationally excited nitrogen oxide fragments obtained from interaction of nitrobenzene vapors with excimer ArF laser radiation. LIF processes of NO in a mixture of nitrobenzene vapors with gases He, Ne, N₂ and atmospheric air are investigated.

1. Experimental Apparatus and Measurement Methods

An electric discharge ArF laser (Coherent, COMPex 102) was used in the experiment on laser radiation interaction with nitrobenzene. Main technical parameters of the laser are shown in the table.

For obtaining narrowband radiation, an optical resonator schematically shown in Fig. 1 was used in the master oscillator (MO). The diffraction grating 2400 grooves/mm was installed in autocollimation mode with second-order reflection. To increase the size of the incident beam before the grating, a prismatic telescope with 10x magnification in one coordinate was used. The laser radiation was output through a rectangular prism with total internal reflection. Part of the prism surface facing the MO had

10% reflectivity, the other part was coated with an anti-reflective layer. Since the spectral linewidth of generation is directly related to divergence of radiation, diaphragm sizes were chosen considering resonator length. To obtain radiation with spectral linewidth 20 pm, beam divergence must be no more than $\Theta = 0.3$ mrad in one coordinate only. Two slit diaphragms sized 6×3 mm were placed along the diffraction grating lines in the selective resonator, which formed a narrowband beam with reduced losses in the vertical section of the beam. To obtain linearly polarized radiation, the laser chamber windows were positioned at Brewster's angle to the optical axis of the resonator. The polarization degree of the output beam at maximum intensity was no more than 0.9.

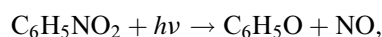
The optical scheme of the experimental setup is shown in Fig. 2. Laser radiation interaction with saturated vapors of nitrobenzene (~ 0.21 Torr) occurred in a stainless steel gas cell at room temperature $T = 298$ K. Quartz windows type KU-1, transmitting with minimal loss the fluorescence of nitrogen oxide in the region 200–250 nm were installed at the window ends of the cell. The cell was pre-evacuated with a turbomolecular pump (ILMVAC, Turbo-V 81-AG) to pressure of 10^{-5} Pa. The experimental mixture of nitrobenzene vapor/inert gas or atmospheric air was introduced into the cell using a mass flow controller (MKS, GE50A013500RMV020). A controlled two-channel pulse generator (Digit-EL, PG-872) was used for the time parameters of synchronization and delays of the recording spectral equipment and the laser source.

Fluorescence registration from excited NO levels NO A²Σ, D²Σ, C²P was performed perpendicular to incident radiation. Quartz lens L collected scattered radiation and focused the interaction zone image onto the entrance slit of the monochromator. Spectral selection of scattered light was carried out by the monochromator (Shamrock, SR-500i) with 500 mm focal length. Temporal and amplitude characteristics of fluorescence were recorded by an iStarICCD camera (Andor Technology, DH720-18F-03) with resolution less than 5 ns at photocathode quantum efficiency $\sim 10\%$ in the region 200–250 nm. The obtained experimental fluorescence spectra of nitrogen oxide were compared with spectral simulation software LIFBase, LIFSim [13,14]. Laser emission energy was measured by a calorimeter (Gentec-EO).

2. Results and Discussion

2.1. Stage of nitrobenzene photofragmentation

For photofragmentation of nitrobenzene, ArF laser radiation with a central wavelength of 193.3 nm was used. The absorption cross-section of nitrobenzene for the incident radiation is shown in Fig. 3. Photokinetic reactions of photofragmentation of nitrobenzene dimer into nitrogen oxides and nitrobenzene monomer are presented as follows [16]:



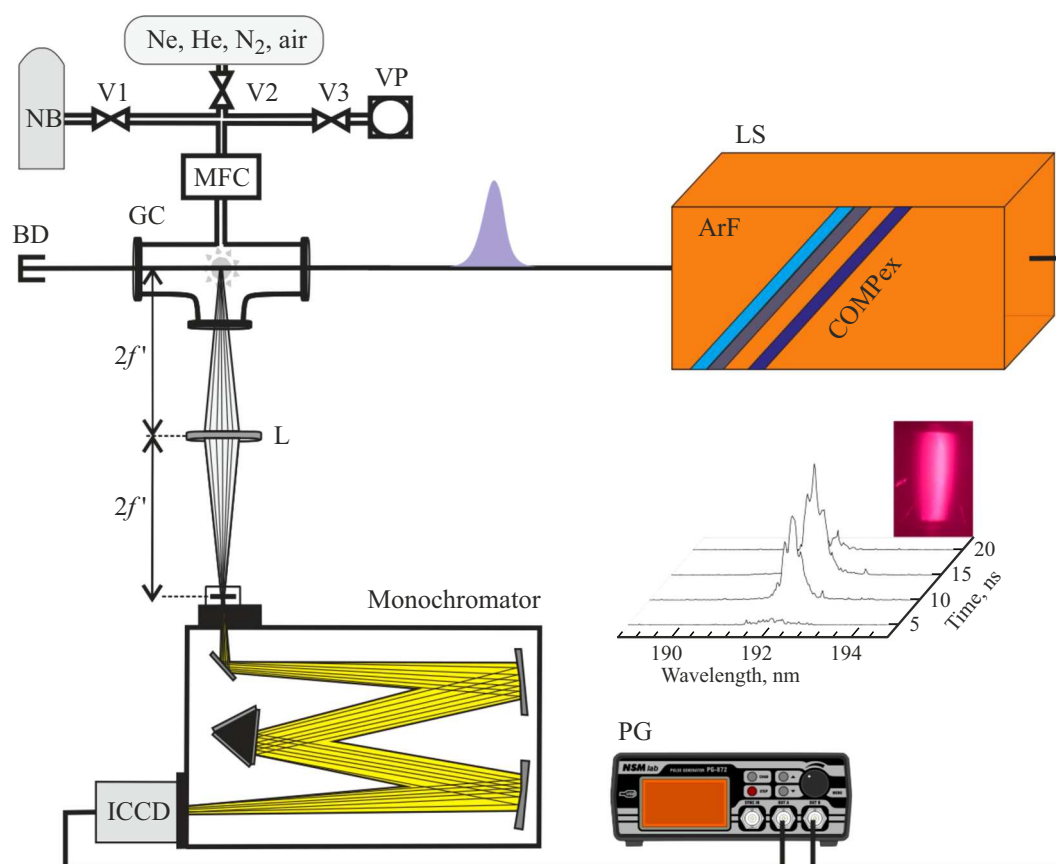


Figure 2. Experimental setup: LS — ArF laser, PG — pulse delay generator, GC — gas cell, BD — beam absorber, L — collecting lens $F = 150$ mm, monochromator with 500 mm focal length, ICCD — intensified CCD camera, MFC — flow controller, V1–V3 — electric valves, VP — vacuum pump.

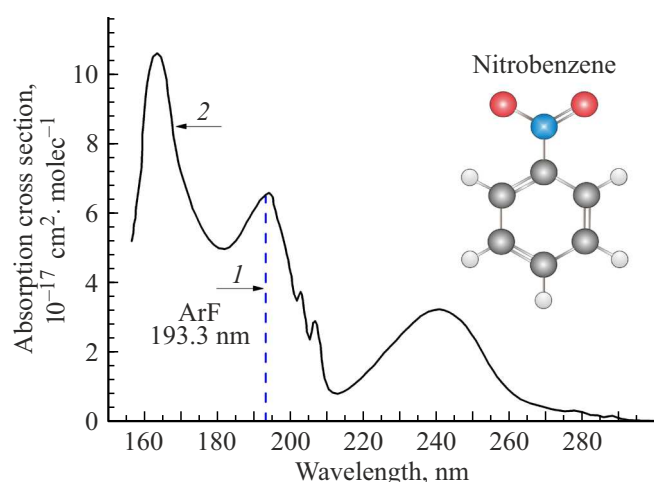
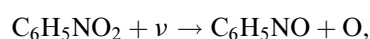
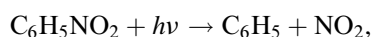


Figure 3. Interaction of laser radiation at 193.3 nm with nitrobenzene: 1 — ArF laser radiation, 2 — experimental absorption cross-section of nitrobenzene [15].

For the subsequent LIF process, reactions (1) and (2) in the model are considered to obtain vibrationally excited states $\text{NO } X^2\Pi$ ($v'' > 0$). The vibrational population of $\text{NO } X^2\Pi$ formed during photofragmentation differs in molecular concentration ratio from the Boltzmann distribution of natural atmospheric $\text{NO } X^2\Pi$ ($v'' = 0/1/2$) — $1/10^{-4}/10^{-8}$ at $T = 300$ K [17]. During the laser pulse duration, the residual energy after nitrobenzene dissociation can be spent on excitation of $\text{NO } X^2\Pi$ and secondary dissociation of NO_2 . By photokinetic channel (1), nitrogen oxide is formed via nitro-nitrate rearrangement ONO , and by channel (2), direct homolytic bond cleavage occurs. Molecules $\text{NO } X^2\Pi, v''$ formed via channel (1) have population distribution over levels $\text{NO } X^2\Pi v''(0/1/2) - (1/0.3/0.1)$ [18,19].

The fragmentation time of nitrobenzene at 193 nm wavelength was calculated in work [20] using quantum-chemical excitation energy calculation by time-dependent density functional theory (TD-DFT). For reaction (1), the time is 900 ps; reaction (2) occurs much faster in 48 ps. During the 10 ns laser pulse at 193 nm, branching of dissociation channels with the product ratio $\text{NO}_2/\text{NO} = 3.125(\pm 37.5\%)$ is ob-

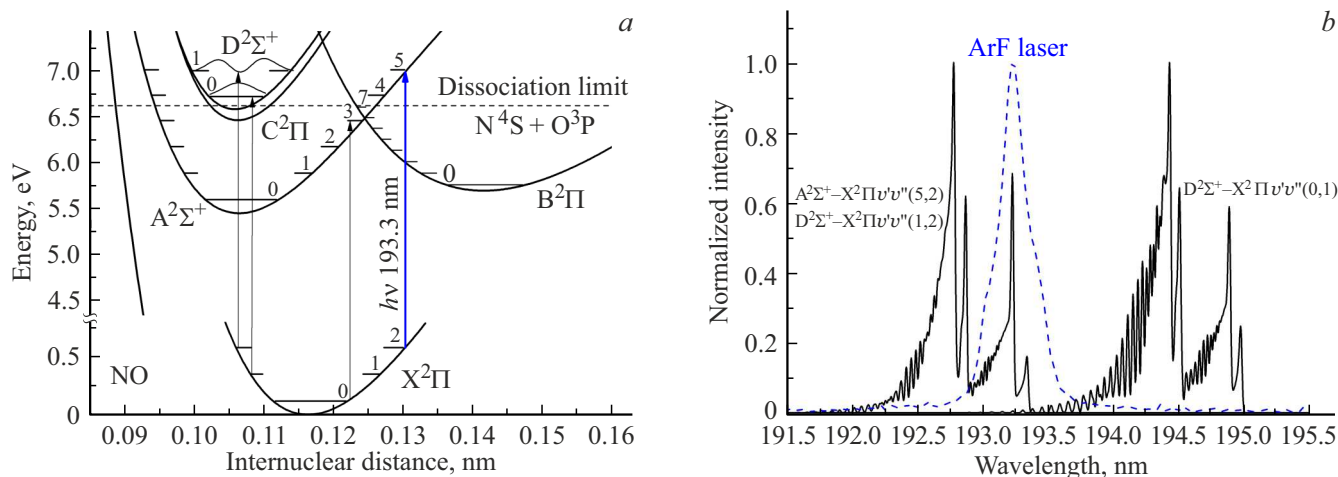
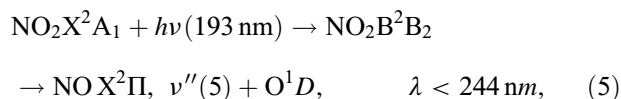
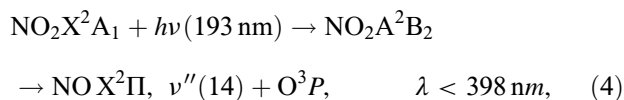


Figure 4. (a) Potential energy curves of NO. (b) Calculated absorption spectrum by LIFBase for NO $A^2\Sigma$, $D^2\Sigma$, $B^2\Pi$.

served. Secondary photodissociation of characteristic NO_2 fragments at 193 nm within 41.8 ps can form vibrationally excited NO $X^2\Pi$, v'' with inverted population [21–25]. The bimodal shape of vibrational population distribution has two maxima — NO $X^2\Pi$ ($v'' = 5$) and ($v'' = 14$) — due to different photokinetic reactions proceeding with varying threshold energies:



3. Laser-Induced Fluorescence of NO $X^2\Pi$

Photon energy of the ArF laser radiation 6.41 eV corresponds to absorption at high rotational levels NO $B^2\Pi - X^2\Pi$ (7,0), $A^2\Sigma - X^2\Pi$ (3,0) and $D^2\Sigma - X^2\Pi$ (0,1), shown in simulated LIFBase spectra in Fig. 4, b. Upon induced excitation of NO $X^2\Pi$ at 0.11 Torr pressure, fluorescence of NO $B^2\Pi - X^2\Pi$ (7, v'') was obtained in [26]. Presence of additional fluorescence transitions NO $A^2\Sigma - X^2\Pi$ (3, v'') and $C^2\Pi - X^2\Pi$ (0,1) in the spectrum is explained by collision-induced redistribution of rotational energy. Weak absorption at transition NO $D^2(v' = 0) - X^2(v'' = 1, J'' = 26.5)$ was reported in [27] upon excitation by ArF laser radiation of NO $X^2\Pi$ molecules at 2 Torr pressure in the cell. Registered fluorescence was compared to the emission spectrum of NO generated in propane flame radiation interactions. In the combustion process at temperature $T = 1750$ K nitrogen oxide is formed via the Zeldovich mechanism. Increase of fluorescence with NO $D^2\Sigma(v' = 0)$ is explained by the growth in population of rotational states NO $X^2\Pi(v'' = 1, J'' = 26.5)$ due to absorption of ArF laser radiation.

Absorption by the subsystem $\Omega = 3/2$ of electronic-vibrational transitions NO $D^2\Sigma - X^2\Pi$ (1,2) and $A^2\Sigma - X^2\Pi$ (5,2) lies at the center of the laser radiation spectral contour. The absorption probability of NO $A^2\Sigma$ at the ArF laser wavelength is higher than that of NO $D^2\Sigma$ judging by absorption coefficients which differ significantly: NO $A^2\Sigma - X^2\Pi$ (5,2) $A_{v',v''} = 1.751 \cdot 10^6$, NO $D^2\Sigma - X^2\Pi$ (1,2) $A_{v',v''} = 1.275 \cdot 10^4$.

The electronic-vibrational energy levels of states NO $D^2\Sigma(v' = 1)$ and NO $A^2\Sigma(v' = 5)$ lie above the dissociation limit NO $X^2\Pi$ 6.496 eV and are close in energy to $\sim 60 \text{ cm}^{-1}$. The lifetimes of these predissociative levels are $16 \pm 1 \text{ ns}$ for NO $D^2\Sigma(v' = 1)$ and $136 \pm 8 \text{ ns}$ for NO $A^2\Sigma(v' = 5)$. Electronic-vibrational transitions to these levels were studied using photoexcitation NO $X^2\Pi$ from the emission line 179.9 nm of an iodine gas discharge lamp. Formation of excited molecules populating levels NO $A^2\Sigma(v' = 5)$ or NO $D^2\Sigma(v' = 1)$ was reported, and fluorescence from the vibrational-rotational level NO $A^2\Sigma(v' = 5, K' = 9)$ was detected. The contribution to fluorescence intensity of energy exchange processes VET between NO $A^2\Sigma(v' = 5)$ or NO $D^2\Sigma(v' = 1)$ was not excluded [28–31]. Through two-photon excitation in fluorescence studies of lower vibrational states NO $A^2\Sigma(v' = 4)$, NO $D^2(v' = 0)$ the possibility of energy transfer was also confirmed NO $A^2\Sigma \rightarrow D^2\Sigma$ [32].

When ArF laser radiation of 20 mJ/cm^2 interacts in a cuvette with saturated nitrobenzene vapor, the obtained NO fluorescence spectrum is compared with modeled LIFBase spectra in Fig. 5. The spectrum was recorded in scanning mode by rotating the monochromator's diffraction grating in 10 nm steps and accumulating the signal over 10 pulses. The integration time set on the camera was 200 ns from the appearance of the laser scattering signal at the unshifted natural frequency. With a larger signal accumulation up to 100 pulses in Fig. 5, a, separated transitions of NO fluorescence NO $C^2\Pi - X^2\Pi$ (0,2) and NO $D^2\Sigma - X^2\Pi$ (1,4) are qualitatively shown. The presence

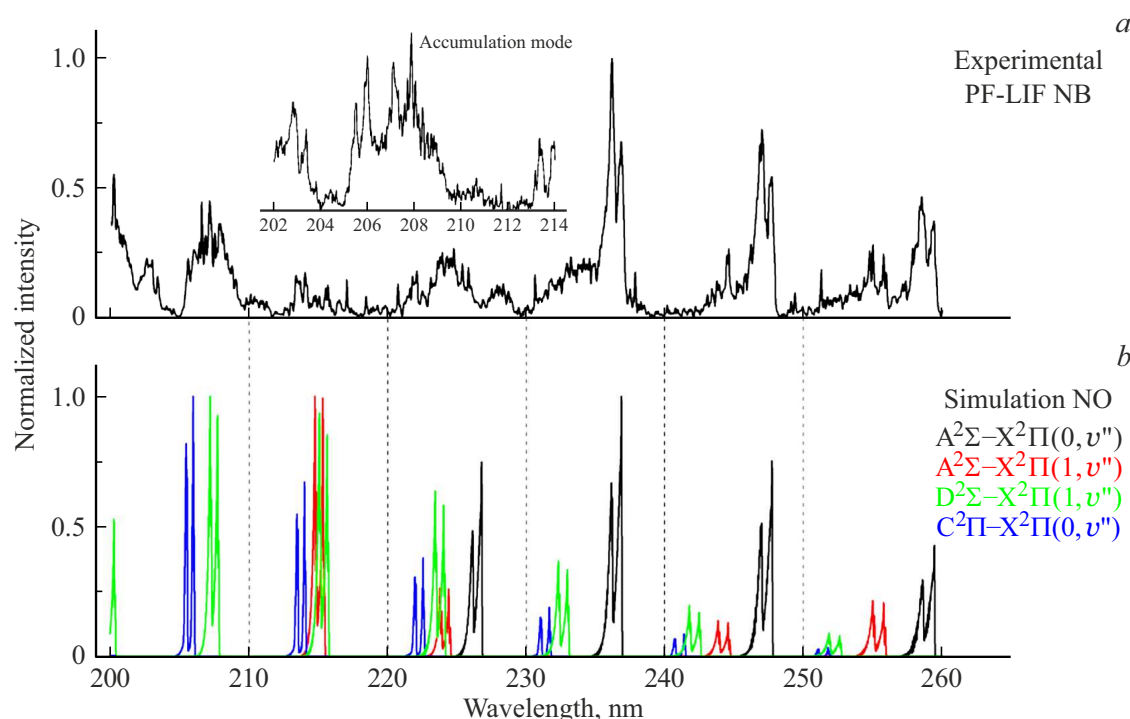


Figure 5. (a) Experimental emission spectrum of NO from the FF-LIF process of nitrobenzene; inset shows transition selectivity in accumulation mode. (b) Calculated LIFBase emission spectrum for NO $A^2\Sigma-X^2\Pi(0, v'')$, NO $D^2\Sigma-X^2\Pi(1, v'')$ and NO $C^2\Pi-X^2\Pi(0, v'')$.

of transitions NO $C^2\Pi-X^2\Pi(0, v'')$ can be explained by heterogeneous interaction between NO $D^2\Sigma(3p\sigma)$ and NO $C^2\Pi(3p\pi)$ due to the similarity of the first orbital and is considered the main deactivation mechanism of NO $D^2\Sigma$ [31,33].

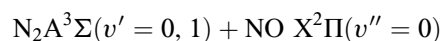
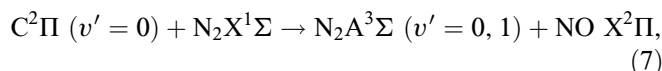
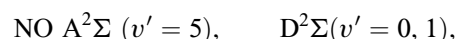
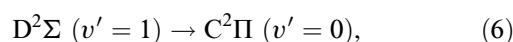
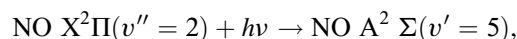
The next factor reducing the emission capability of the NO $D^2\Sigma$ state is the relaxation of states NO $D^2\Sigma(v' = 1)$ and NO $C^2\Pi(v' = 0)$ due to optical radiative transitions. It is known that experiments using synchrotron radiation and pulsed laser photolysis at 165 nm registered transitions NO $D^2\Sigma-A^2\Sigma(1,1)$ at wavelength 1.069 μm and NO $C^2\Pi-A^2\Sigma, v'v''(0,0)$ — 1.22 μm [34–36]. Oscillator strengths of the cascade relaxation mechanism were experimentally determined for transitions NO $C^2\Pi-A^2\Sigma$ at $f_{os} = 0.7$ and NO $D^2\Sigma-A^2\Sigma$ at $f_{os} = 0.18$ consistent with the intensity of observed NO $A^2\Sigma-X^2\Pi(0-1, v'')$ emission [37]. Practically, the cascade photoexcitation mechanism of NO $A^2\Sigma \rightarrow D^2\Sigma$ in the range 1.06–1.15 μm allowed effective signal selection by two-photon LIF during interaction of far UV-C laser radiation with atmospheric nitric oxide [38].

Fig. 6, a shows a kinetic series of part of the NO $D^2\Sigma$ and $A^2\Sigma$ fluorescence spectrum during FF-LIF of nitrobenzene in a cuvette at $T = 298\text{ K}$. The observed emission time around 208 nm is about 35 ns, exceeding the radiative lifetime of NO $D^2\Sigma$ equal to 18 ns, and the 10 ns laser pulse duration. The experimentally measured fluorescence duration, longer than the NO $D^2\Sigma$, lifetime, may indi-

cate energy exchange in NO $A^2\Sigma \rightarrow D^2\Sigma$. The radiative transition NO $D^2\Sigma-X^2\Pi(1,4)$ at $k_{em} = 4.927 \cdot 10^6\text{ s}^{-1}$ occurs much faster than transition NO $A^2\Sigma-X^2\Pi(0,2)$ at $k_{em} = 6.774 \cdot 10^5\text{ s}^{-1}$.

Fig. 6, b shows quenching of arising NO fluorescence in mixtures of nitrobenzene vapor and different gases at a total pressure of 1 atm. The strongest quenching in obtained spectra occurs in atmospheric air. Studies of lower excited vibrational levels show oxygen has large quenching rate constants: $k_Q = 5.4 \pm 0.22 \cdot 10^{-10}\text{ cm}^3\text{mol}^{-1}\text{s}^{-1}$ for NO $D^2\Sigma(v' = 0)$ and $k_Q = 1.6 \pm 0.2 \cdot 10^{-10}\text{ cm}^3\text{mol}^{-1}\text{s}^{-1}$ for NO $A^2\Sigma(v' = 0-4)$ [30,32,39].

In the case of a nitrogen environment in the cuvette, there is a significant increase in NO $A^2\Sigma(v' = 0)$ fluorescence due to electronic (EET) and vibrational (VET) energy transfer processes [40,41]:



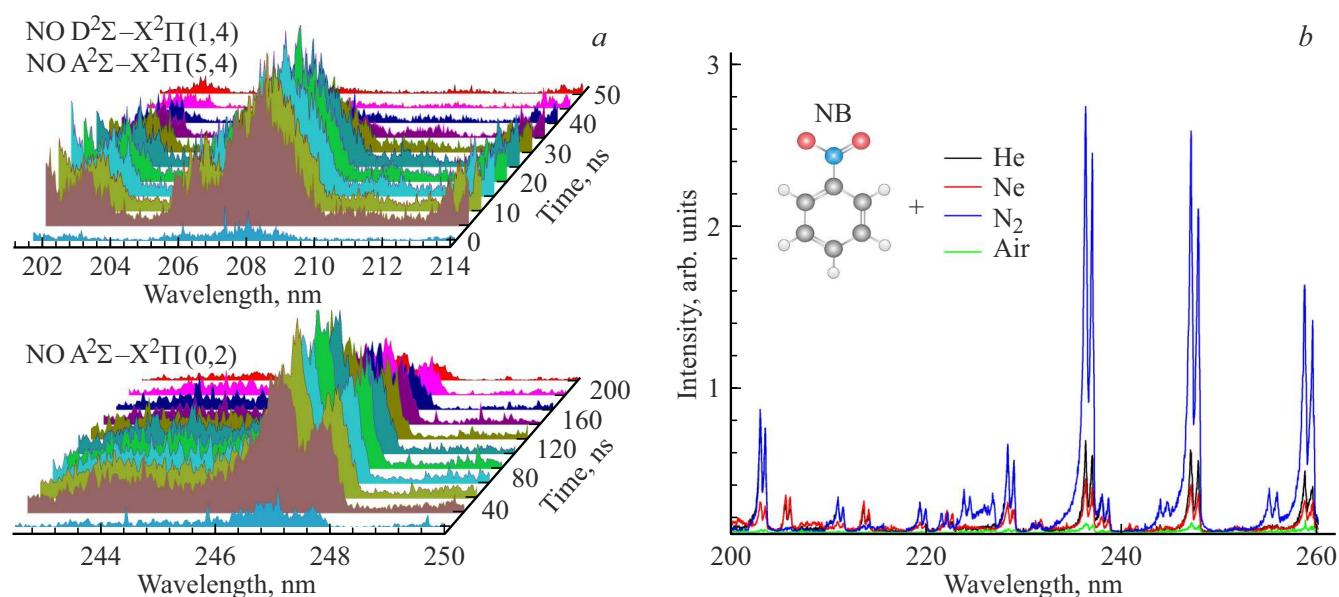


Figure 6. (a) Kinetic series of emission spectra of NO $A^2\Sigma-X^2\Pi$, $v'v''(0,2)$ and $v'v''(5,4)$. (b) Emission spectrum of NO in an environment of various gases.

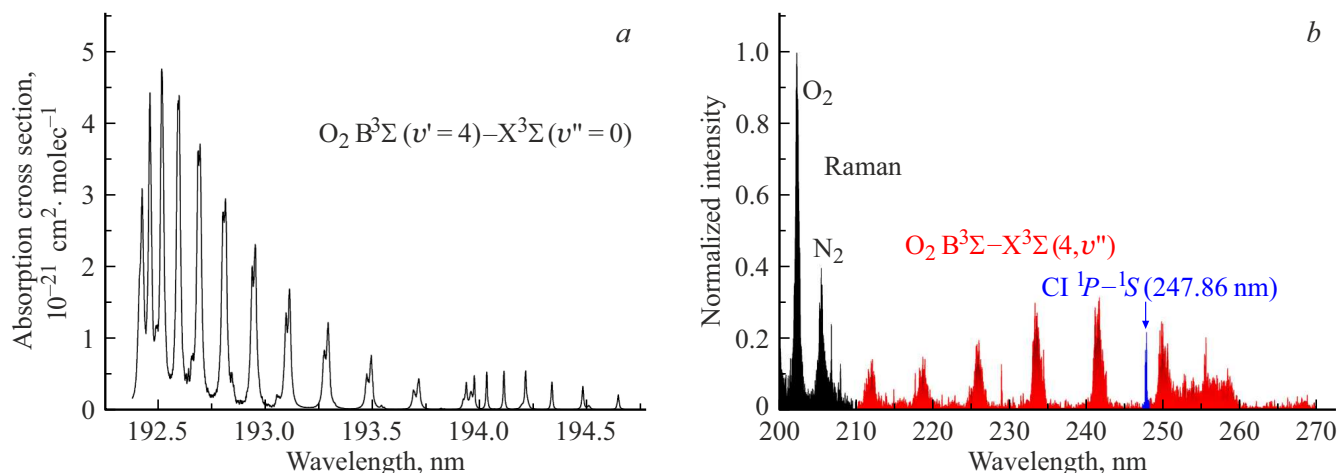


Figure 7. (a) Absorption spectrum of $O_2 B^3\Sigma(v'=4)-X^3\Sigma(v''=0)$ [42]. (b) Fluorescence spectrum of air at atmospheric pressure, excited by ArF laser radiation.

Since direct optical excitation of the $N_2 X^1\Sigma$ ground state to the $N_2 A^3$ electronic level is forbidden by spin-orbit interaction, only collisional deactivation of highly excited NO levels is possible. Molecules $N_2 X^1\Sigma$ quench excited NO states $A^2\Sigma$, $D^2\Sigma$ and $C^2\Pi$ at $k_Q(7) = 2.6 \pm 0.2 \cdot 10^{-10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ forming $N_2 A^3\Sigma(v'=0,1)$. This process results in nonradiative electronic-vibrational energy transfer to $NO A^2\Sigma(v'=0-2)$ at $k_{ET}(8) = 15 \pm 3 \cdot 10^{-10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ with vibrational level population ratio 1.0 : 0.15 : 0.014 [32,42].

It is known that ArF laser radiation in atmospheric air induces concomitant fluorescence of the Schumann-Runge bands— $O_2 B^3\Sigma v'(4) - X^3\Sigma v''(0)$ [26,27,43,44]. For the transition $NO A^2\Sigma-X^2\Pi$, $v'v''(0-3,0)$ absorption cross

sections were experimentally precisely measured in the interval from $(1-3) \cdot 10^{-18} \text{ cm}^2 \text{ mol}^{-1}$ using various methods [45,46]. According to LIFBase calculated coefficients for the vibrationally excited NO $A^2\Sigma-X^2\Pi v'v''(5,2)$ transition, the absorption cross section is approximately 10^{-18} . Fig. 7, a shows oxygen absorption cross section for laser central wavelength 193.34 nm with spectral width 300 pm falls within $4.5 \cdot 10^{-23} - 7.01 \cdot 10^{-22} \text{ cm}^2 \text{ mol}^{-1}$ substantially less than that of nitric oxide. To obtain oxygen fluorescence $O_2 B^3\Sigma$ laser energy density was increased to 100 mJ/cm^2 (Fig. 7, b). At this energy density, spontaneous combination scattering of oxygen and nitrogen is registered in the spectrum. The fluorescence spectrum also shows atomic carbon C I, formed via interactions with CO_2 in atmospheric

air. Study [26] determined oxygen fluorescence lifetime $O_2\ B^3\Sigma\ (v' = 4)$ as 10^{-12} s, allowing time-based selective detection of nitric oxide fluorescence with faster registration systems.

Conclusion

Processes of interaction of far UV-C laser radiation with nitrobenzene vapor phase using FF-LIF method were considered. After photofragmentation of the parent molecule, laser-induced excitation occurs not only of $NO\ D^2\Sigma - X^2P\ (1,2)$ but also $NO\ A^2\Sigma - X^2P\ (5,2)$. Molecular nitrogen was found to enhance fluorescence of $NO\ A^2\Sigma\ (v' = 0)$ state via VET energy transfer to metastable level $N_2\ A^3\Sigma$ during quenching of $NO\ D^2\Sigma$ and $A^2\Sigma$.

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Conflict of interest

The authors declare that they have no conflict of interest.

Author contributions

A.V. Puchikin: conceptualization, conducting the study, writing; Yu.N. Panchenko: administration, text editing, final approval; M.V. Andreev: statistical data processing; V.E. Prokopyev: statistical analysis, methodology development.

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