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B-21

APPLICATION OF TIME-RESOLVED FLUORESCENCE SPECTROSCOPY TO PROTEIN STRUCTURE

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The fluorescence spectroscopy is a very sensitive technique to monitor the changes in protein structure during the different biochemical processes. Typically, tryptophan residues are used as an intrinsic fluorescent probes in proteins due to a high degree of sensitivity to their local environment, including polarity and viscosity. However, the fluorescence spectra and lifetimes for multi-tryptophan proteins are difficult to interpret unambiguously, since the single tryptophan proteins have at least two lifetimes. In this work, we applied the time-resolved spectroscopy to analyze the fluorescence lifetimes and corresponding decay associated spectra for proteins with different number of tryptophan residues upon conformational changes.

The fluorescence decays of four proteins were fitted by three lifetimes both for native folded conformation ($\tau_1 = 5.4\text{--}7.0$ ns, $\tau_2 = 1.3\text{--}2.3$ ns, $\tau_3 \leq 0.1$ ns) and for unfolded protein ($\tau_1 = 4.4\text{--}5.0$ ns, $\tau_2 = 1.7\text{--}2.0$ ns, $\tau_3 \leq 0.05$ ns). It was shown that it is not the absolute value of the tryptophan fluorescence lifetime that depends on the specific structure of a protein, but rather the relative contribution of the decay-associated components. For unfolded proteins, irrespective of their initial structure, the time-resolved spectra and relative contributions of lifetime components became similar. The lifetime components were compared with a classification of tryptophan residues in the structure of these proteins within the discrete states model. Based on the data that were obtained by time-resolved fluorescence spectroscopy, we were able to resolve the fluorescence spectrum of the multi-tryptophan protein into components that correspond to different tryptophan groups that are present in its structure. The spectrum of the long lifetime component τ_1 is bathochromically shifted, indicating that the tryptophan residues of this group are accessible to bulk water because of high polarity and mobility in their local environment. The result of this work can be further employed to investigate the stages of protein unfolding/folding and the involvement of different protein domains in its conformational dynamics that are associated with catalysis.

B-22

INTERMOLECULAR PROTON TRANSITION IN THE EXCITED STATES OF ACRIDINE

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In the present report results of theoretical studying of the acid-base properties of acridine in different electronic states are presented. Numerous experimental measurements show, that at transition from the ground state in S_1 a $\pi\pi^*$ -state basicity of acridine considerably increases. Estimations were spent by the Ferster techniques. A number of researchers calls these results into question. For example, A. Terenin specified, that at excitation resolution occurs and, means, entropy can essentially change [1]. It is feature it is not considered at calculations by the Ferster techniques. Experimental basicity T_1 state (the same orbital nature, as S_1 , and the same distribution of electronic density) is close to basicity of a S_0 state. It too brings doubts as basicity does not depend from state multiplicity.

Our calculations (estimations using MEP) also testify to close basicity of all three states [2]. At the analysis of results of calculations it has been established, that basicity in $S_3\pi\pi^*$ - state strongly increases (values MEP). S_1 and S_3 states are also connected by strong internal conversion, i.e. by strong electron-vibrational interaction. It does possible borrowing of basicity of S_1 state from S_3 state.

Features of intermolecular proton transition (basicity) in the electronic excited states of acridine taking into account the borrowing mechanism are discussed.

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B-23

SPECTRAL-LUMINESCENT AND PROTON-ACCEPTOR PROPERTIES OF BIOLOGICALLY ACTIVE HYDROXYL-SUBSTITUTED BENZALDEHYDES

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Using methods of electronic spectroscopy and quantum chemistry (INDO method) the electronic structure and spectra of some hydroxyl-substituted benzaldehydes have been investigated. Comparison of accuracy of the description of spectral-luminescent properties and intramolecular photophysical processes in the isolated molecules received in calculations and experiments is spent. Influence of hydroxyl and tret-butyl substitution on distribution of electronic density and proton-acceptor ability of molecules in the basic electronic state is considered.

Possibilities of investigated derivatives to form intra- and intermolecular hydrogen bonds are estimated. The substitutes entered in phenol fragment of investigated molecules, make various impact on proton-acceptor ability of derivatives of benzaldehyde. Thus appreciable influence renders not only a replacement place, but also a spatial structure of substituting fragments. Correlation between value of MEP, connected with hydroxyl substitutes, and antiviral activity of compounds under investigated, estimated on cell culture of viruses of a herpes of flu [1] is established.

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B-17

LUMINESCENCE PROPERTIES OF HEAVILY DOPED ALGAN FILMS UNDER OPTICAL AND ELECTRON BEAM EXCITATION

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Spectral characteristics of spontaneous and stimulated luminescence were investigated from the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{AlN}$ solid solutions with Si dopant concentration more than 10^{20} cm^{-3} at $x = 0 \dots 1$, which were grown by molecular beam epitaxy on sapphire substrates. The excitation of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ films was carried out by pulsed laser radiation ($\lambda = 266 \text{ nm}$) from the Nd: YAG laser with a power density of up to 9 MW/cm^2 and an electron beam with an electron energy of up to 20 keV and the current of up to 100 A , formed in an "open" discharge. Figure (a, b) shows typical spectra of spontaneous photoluminescence – (a) obtained at an angle of 45° to the surface and cathodoluminescence spectra from cleaved edges of the structure – (b).