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B-23

MODELING OF SPECTRA AND LASING EFFICIENCY WITH CHANGING CONCENTRATION OF CHROMENES AND PUMP POWER DENSITY

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Using the previously developed model describes the physics of photoprocesses in complex organic compounds [1, 2] simulations of lasing in the active media based on chromium-3, chromium-13 and their julolidine analogues at pulsed laser pumping was carried out. Curves generating efficiency depending on the density of the pump power and the concentration of the dye in the active medium were plotted. It is shown how in this case varies spectrum of stimulated emission. The course of the experimental curves of the efficiency on the pump power density was confirmed.

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B-24

SPECTRAL-LUMINESCENT PROPERTIES OF MEROCYANINE DYES DERIVED FROM BENZOXAZOLE

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Merocyanine dyes based on the benzoxazole nucleus are used as fluorescent probes, active laser media, sensitizers for photodynamic therapy. Direct search of new merocyanine dyes with consciously known properties requires finding the dependence their spectral-luminescent properties on the structure and the medium nature. In this work regularities of these properties were investigated in solvents of different polarity according to the polymethine chain length and the electron-acceptor ability of the endgroups of dyes derived from benzoxazole. Ab initio quantum chemistry methods were applied to analyze the electronic structure.

It was found that with increasing electron-acceptor ability of endgroup in the row malononitrile-barbiturate-thiobarbiturate, the electronic structure of merocyanines changes smoothly in the direction of the ideal limit structures: neutral polyene – polymethine – bipolar polyene. This tendency enhances with increasing the polymethine chain length. Such variation of the electronic structure of dyes allowed achieving of the positive, negative and reversible solvatochromism. It is shown that variation polarity of the solvent also affects the ratio of the polyene-polymethine electronic states. It was found a nontrivial effect – record fluorescence quantum yields of dyes with rigidly loose polymethine chain, which is the main channel of radiationless deactivation of the excited state.