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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 tert-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).