

Electronic properties of polymethine systems. 10. Electron structure and absorption spectra of cyanine bases

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Abstract

Complex quantum-chemical and spectral studies of the features of the electron structure and absorption spectra of the bases' derivatives of the symmetrical cyanine dyes are performed. It is found that moving from cationic cyanines to their neutral bases is accompanied by a drastic increase in the bond length alternation, equalizing the electron densities at atoms in the chromophore and by sharp shifting up of the molecular levels. Spectral bands in the absorption spectra of the bases are essentially wider and lower intensive and hypsochromically shifted, what is suggested to be connected with different nature of the first electron transition in the cyanine dyes and their bases.