Electronic properties of polymethine systems. 11. Absorption spectra and nature of electron transitions in cationic oxystyryl and their neutral derivatives

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Abstract

Complex quantum-chemical and spectral study of the features of the electron transitions and absorption spectra of the both oxystyryls and related merocyanines containing the pyridinium, quinolinium, indolium and benz[*c*,*d*]indolium end residues has been performed. It was shown that the relative long wavelength absorption of the neutral merocyanines, in comparison with the cationic dyes, is caused by considerable redistribution of the electron density within the chromophore upon excitation, not by equalizing of the carbon–carbon bond lengths as it was predicted in the framework of the conception "cyanine limit". The opposite sign change of the dipole momentum in the excited state in the cationic and neutral dyes depends noticeably on the basicity of the donor end groups and causes the opposite solvatochromism which increases additionally the distance between the absorption bands of these dyes of the different types.