INVESTIGATION OF CHARGE WAVES IN THE CHROMOPHORE OF CATION CYANINE DYES USING ^{13}C NMR SPECTROSCOPY

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S u m m a r y

The electron density distribution for a series of symmetric and non-symmetric cation cyanine dyes is investigated on the basis of the data of quantum-chemical calculations and NMR (^{13}C) spectra. It is shown that the calculated atomic charges are in good agreement with the experimental values of chemical shifts. A considerable wave-like alternation of the electron density along the chromophore is found. It is shown that the general electron density distribution represents a superposition of the autolocalized charge and two charge waves generated by the donor finite groups.