

## ELECTRONIC STRUCTURE AND ABSORPTION SPECTRA OF CYANINE DYES DERIVED FROM TETRAZOLOISOINDOLES

We have made quantum-chemical calculations of electronic structure and spectral data for cyanine dye by Pople-Pariser-Parr method, which is most suitable in case of cyanine dyes.

As parameters for PPP calculations we used ionization potentials for Carbon and Nitrogen atoms  $I_C=11.16$  eV,  $I_N=14.12$  eV and homocentric integrals for interactions of p-electrons  $\gamma_{CC}=-6.20$  eV,  $\gamma_{NN}=-7.20$  eV. As for two-centered integrals we used Mataga-Nishimoto approximation. It is accepted that methyl group has not significant influence. Bond length and valence angles were used at standard values, except for valence angle near Carbon atom at meso position was increased to 130° accordingly to references. Similarly to other work, we used configurational interactions of 4 mono-excited states.

For our substance we have found absorption maximum at long-wave band 557.0 nm, which correlates with experiment, and oscillator strength  $f=0.531$ . Oscillator strength characterizes intensity of the absorption band and can be compared to the absorption extinction  $\epsilon$  for this dye ( $\lg \epsilon=4.86$ ).

Accordingly to the calculated  $\pi$ -charges and order of  $\pi$ -links at ground and first excited states, at ground state Carbon atom at meso-position has significant positive charge (0.116-0.118 e), which correlates with references, and in excited state electron density increases, which leads to the negative charge (-0.165÷-0.169).

In case of R=H molecule has  $C_{2v}$  symmetry. Its HOMO refers to  $A_2$  group, thus being asymmetric to the plane  $\sigma_V(xz)$ , and its LUMO refers to  $B_1$  group, thus being symmetric to the plane  $\sigma_V(xz)$ . So, electron transition  $A_2 \times B_1 = B_2$  is permitted and polarized along chromophore axis (axis y). Therefore this transition must correspond to the intense absorption band, which correlates with the experiment.

Key words: cyanine dyes, tetrazoloisoindole, Ilchenko's scale.