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Prediction of vertical ionization potentials for organic compounds by integral characteristics of optical spectra and the number of protons in molecules

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Abstract

In this review, the authors summarize the results of the first vertical ionization potentials with the structural and spectral integral descriptors of organic compounds: the integral oscillator strength defined in the visible or UV regions of the spectrum and the total number of protons in organic molecules. The adequate non-linear regression models relating the potentials of ionization as functions of the integral oscillator strength in the range between 6.53 eV and 1.63 eV (from 190 to 760 nm) and the total number of protons in organic molecules. The regularities were allowing to estimate the first ionization potentials for organic oxygen – and nitrogen-containing compounds established. The established regularities are interpreted as the influence of exchange and electrostatic interactions on the energies of the highest occupied molecular orbitals. The ionization potentials were calibrated according to the method of Hartree-Fock (RHF) method using 6-31G(d,p) basis set from the Koopmans' theorem. The obtained models allow us to estimate first ionization potentials of organic oxygen-and nitrogen-containing molecular systems by the integral oscillator strength and by the number of protons with an accuracy of 0.4 to 9%. This accuracy is quite suitable for practical applications. The research results can be used in chemistry, photochemistry, molecular electronics, photonics, and physical chemistry to study electron transfer processes, the characteristics of the band structure of nanoparticles. The present paper examples confirmed by statistical data processing.

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