Thematic Section: Theoretical Research. **Full Paper**
Subsection: Physical Organic Chemistry. *The Reference Object Identifier* – ROI: jbc-01/19-57-1-1
The Digital Object Identifier – DOI: 10.37952/ROI-jbc-01/19-57-1-1
Submitted on January 17, 2019.

Integral characteristics of optical spectra, as a new class of descriptors for complex molecular systems

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Keywords: descriptors, structure-properties, spectrum-properties, electronic structure, molecules, molecular systems, biological fluids, hydrocarbon mixtures.

Abstract

The authors summarized the results on the study of the relationship of physicochemical properties with spectral integral characteristics of complex molecular systems: integral absorption, reflection coefficients, integral oscillator forces, color characteristics, integral autocorrelation functions, signal convolutions defined in the visible or UV spectral regions.

It is shown that these integral characteristics are numerical parameters that adequately convey the physicochemical and electronic properties of molecules and their mixtures, so these values can be used as descriptors. Since electronic spectra are unique characteristics of a substance, these descriptors have a high discriminating ability. The classification of such descriptors is given. These values differ from physicochemical descriptors such as absorption maxima, since their determination requires information on the spectrum of these systems without isolating individual bands and maxima using the Fourier transform. In contrast to conventional physicochemical and quantum mechanical descriptors, the proposed descriptors can be applied to the study of multicomponent systems with unknown structure and composition. This makes it possible to use these values to determine the physicochemical properties and averaged over the composition of the electronic characteristics of a substance, such as petroleum distillates, petroleum, biological fluids, and similar mixtures. The paper provides relevant examples, confirmed by statistical data processing. The obtained patterns should be defined as the patterns "spectrum-property" by analogy with the patterns "structure-property", known in organic chemistry and chemical informatics. The consistency of the developed approach is shown, and a quantum-chemical interpretation of these laws is given. Based on the established spectrum-property dependencies, analytical methods can be developed for determining the amount of complex hydrocarbon systems, such as oil and their products, gas condensates, products of high-temperature pyrolysis of organic substances, etc. The established patterns can be applied to determine the ionization potentials and electron affinity of molecules, as well as in medical diagnostics, oil refining, petrochemistry, oil field development technology, and other fields of science and nanotechnology.

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