

An attempt to quantitatively describe the relationship of properties of the compound on its chemical structure by A.M. Butlerov

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On the 150th anniversary of the theory of chemical structure of organic compounds

Abstract

In this article some of the key provisions A.M. Butlerov's theory of chemical structure of organic compounds and their implementation in modern statement are given in the historical aspect. It focuses on communication Butlerov postulate properties of compounds with the structure. In accordance with A.M. Butlerov's proposals we can quantitatively describe the chemical structure of an organic compound by independent descriptors of three types: topological, which can act as one of the topological indices, such as Wiener index, the geometric and electronic ones. As a geometric descriptor there has been suggested the moment of inertia of rotational motion J or its feature of $MW^{2/3}$. Descriptor J does not depend on the topological index. Its advantage and independence lies in the fact that the order of binding atoms to each other is not important. It can be used to describe both the classical molecules, and katenats, dimers, associates of supramolecular compounds, complexes, which act as independent kinetic entities in the manifestation of reactivity and properties. As the electronic index there is taken ionization potential and affinity to electron. In accordance with this, the basic postulate of the theory is the dependence of y_i properties on the structure, – it can be written as $y_i = f(W, J \text{ or } J_w, PI, A_E)$. In the article there are given a few examples of using the given dependence.

"Nowadays, after discovering a whole mass of unexpected and important facts, almost everybody is aware that theoretical side of chemistry does not correspond to its real development".

A.V. Butlerov