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About the connection of the activation energy of the chemisorption of direct dyes with the topological characteristics of their molecules

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Abstract

This paper investigates the macrokinetic behavior of sorption of direct dyes on fibers of the cellulose material. Quantum-chemical calculations using the density functional method (B3LYP) with a basic set of 6-31G** found that the molecular forms of these dyes are non-planar. A two-parameter topological descriptor describing the relationship between the structure and macrokinetic characteristics of dye molecules is proposed. The relationship between the sorption activation energy of the dye and topological characteristics of molecules, which indicates the role of structural and chemical effects, is established. We consider as topological characteristics the simple Wiener index and dispersion of huckel energies, which reflect the eigenvalues of a topological matrix. The Wiener simple index and the Hückle energy dispersion, which reflects the eigenvalues of the topological matrix, are considered as topological characteristics. The variance of the sum of squares of the eigenvalues of the Hückel matrix characterizes fluctuations of the spectrum of the energy states of the molecule. The simple Wiener index takes into account heteroatoms, but does not take into account multiple and aromatic bonds. It is assumed in the work that the enthalpy energy component in the series of the molecules under consideration reflects the dispersion of the Hückel energies, and the entropy energy component reflects the Wiener index. It is shown that there is a correlation between the Wiener indices, the dispersion of the spectrum of the Hückel energy states of the dye and the activation energy of sorption of the direct dye, which indicates the orbital control of the sorption of direct dyes in the direct dye-fiber system of cellulose tissue and the possibility of charge transfer from the dye to the active centers of the fiber. The obtained correlation shows that the activation process of sorption is associated with overcoming steric hardships. A similar approach can be used in organic chemistry for the directed synthesis of large organic molecules containing heteroatoms.

References

[1] B.N. Melnikov, T.L. Scheglova, G.I. Vinogradova. Application of dyes: the manual for higher schools, 3rd ed. BINOM. *Knowledge laboratory, Moscow.* **2014**. 331p. ISBN 978-5-9963-0232-1 (russian)
[2] F.J. Duarte and L.W. Hillman (Eds), Dye laser principles. With applications. *Academic Press Inc, New York.* **1990**. 456p.
[3] M.Yu. Dolomatov, K.I. Kobrakov, E.A. Kovaleva. *Bashkir chemical journal*. **2005**. Vol.12. No.4. P.42-44. (russian)
[4] M.Yu. Dolomatov, T.M. Aubekerov. *Russian Journal of Physical Chemistry A*. **2018**. Vol.92. No.3. P.401-406. (russian)
[5] M.Yu. Dolomatov, E.A. Kovaleva, D.A. Khamidullina. *Russian Journal of Physical Chemistry A*. **2018**. Vol.92. No.5. P.943-947. (russian)
[6] M.Yu. Dolomatov, A.V. Kutueva, E.A. Kovaleva, and N.A. Zhuravleva. Relationship between macrokinetic parameters thermolysis process and topological characteristics for hydrocarbons molecules. *Butlerov Communications.* **2018**. Vol.55. No.8. P.59-65. DOI: 10.37952/ROI-jbc-01/18-55-8-59
[7] Chemical application of topology and graph theory. Ed. R. King. *Mir Publ., Moscow.* **1987**. 560p. (russian)

[8] Norman R. Draper. Harry Smith Applied Regression Analysis, 3rd Edition. *Wiley & Sons Inc, New York.* **1998**. 736p. ISBN 0471170828
[9] N.S. Zefirov, S.I. Kuchanov (Eds.). Applications of Graph Theory in Chemistry. *Nauka, Novosibirsk.* **1988**. 306p. (russian)
[10] Streitwieser. Molecular Orbital Theory for Organic Chemists. *John Wiley & Sons, Inc, New York.* **1961**. 489p.
[11] E.A. Kovaleva, M.Yu. Dolomatov. Kinetics features of dyes interaction with fibrous materials: textbook. *Ufa State Institute of Service. Ufa.* **2005**. 78p. (russian)