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π-ELECTRON AFFINITY OF NITROGENOUS CONJUGATED HETEROCYCLES

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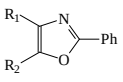
Conjugated heterocycles continue to apply in a practice because of their π-electron system; so, they use widely as special functional components of biological active molecules and drugs (pharmacophors). The branched collective system of π-electrons enables to generated the stable complex ***[pharmacophor] – [biological active center of proteins]***. Here, we propose treat an ability of the conjugated system to generate the π-complex as an π-electron affinity. For the quantitative estimation of this property, the relative position of the frontier levels can be used. Earlier, we have proposed to characterize the relative positions of the frontier levels in any conjugated molecules by the following index φ_0 [1]. Thus, the index φ_0 could be apply for the donor/acceptor π-electron affinity of the conjugated nitrogenic heterocycles to estimate quantitatively. The important attention is attended the biological active conjugated heterocycles which can be tested as effective pharmacophors: in this case, the index φ_0 could be treated *biological π-electron affinity.* This work presents the caculated index φ_0 for some simplest mono- and bicyclic heterocycles, nucleic bases as well as for oxazoles with donor and/or acceptor substituents **1-6**.

Table. Energies MO and index φ_0 in oxazoles 1-6 (in eV)

	R_1	R_2	ε_{HOMO}	ε_{LUMO}	φ_0
1	CN	$N(CH_3)_2$	-6.72	0.12	**0.53**
2	CN	S-CH_3	-8.33	2.24	**0.54**
3	CN	S-Ph	-8.56	2.13	**0.53**
4	SO_2Ph-CH_3	S-CH_3	-8.30	2.25	**0.55**
5	CN	SO_2CH_3	-9.38	1.43	**0.46**
6	SO_2Ph-Me	SO_2CH_3	-9.18	-0.06	**0.38**

The *in vitro* studies are consistent with the following conclusion: compounds with donor substituents **1-4** do not exhibit inhibitory properties, and compounds with acceptor substitutions **5-6** exhibited a clear inhibitory effect on cancer cell growth [2].

[1] O. Shablykin, O. Kobzar, Ya. Prostota, O. Kachkovsky, V. Brovarets, A. Vovk, D. Merzhyievskyi, N. Obernikhina. Topological Index of Electronic Structure of Conjugated Substituted Bis-Oxazoles and Their Spectral-Luminescent Properties. //Electronics and Nanotechnology (ELNANO-2018): Proc. of 38th Int. Sci. Conf.– Kyiv, 2018. – PP. 449 – 453.

[2] M. V. Kachaeva, D. M. Hodyna, I. V. Semenyuta, S. G. Pilyo, V. M. Prokopenko, V. V. Kovalishyn, L. O. Metelytsia, V.S. Brovarets. Design, synthesis and evaluation of novel sulfonamides as potential anticancer agents.Comp. Biol. Chem.-Vol.74, 2018, – PP. 294 – 303.