

# Topological Index of Electronic Structure of Conjugated Substituted Bis-Oxazoles and Their Spectral-Luminescent Properties

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## Abstract

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### Abstract:

The study of effects caused by the conjugated bridge binding of heterocycles (forming of  $\alpha,\omega$ -disubstituted polyenes) was performed by quantum-chemical and spectral methods. It is shown that such modification of chemical constitution is accompanied by essential changes in the donor-acceptor property and energy gap. For the quantitative estimation of the influence of substituents on the donor-acceptor characteristic, the topological index  $\varphi_0$  is used. Also, the spectral effects of the substituents on the energy gap were studied; they were experimentally observed in the spectra of the heterocycles and their bridged derivatives.

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