

## On peculiarities of naphtho- and anthrathriazoleoxides formation from 2-azido-3-(*N*-alkyl-*N*-nitrosamines)-1,4-naphthoquinones and 3-(*N*-alkyl-*N*-nitrosamine)-5-arylamino-6*H*-6-oxo-anthra[1,9-*cd*]isoxazoles

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### Abstract

For in-depth study of the formation of the 3-alkylamino-5-arylamino-6*H*,11*H*-6,11-dioxoantra [1,2-*d*][1,2,3]thiazole-2-oxides from 3-alkylamino-5-arylamino-6*H*,6-oxoantra[1,9-*cd*]isoxazoles we carried out the synthesis of 3-(*N*-alkyl-*N*-nitrosoamino)-5-(*p*-toluidino)-6*H*-6-oxoantra[1,9-*cd*]isoxazoles. The results of UV and NMR spectra indicate that *N*-nitroso compounds isomerization in thiazoleoxides does not include the formation of nitrenes, and proceeds, apparently, according to the agreed mechanism. The carried out quantum-chemical calculations allowed us to estimate the thermodynamic parameters of these reactions in the gas phase and in solution in the approximation of PCM. It is shown that all the investigated reactions are thermodynamically favorable both in the gas phase and in solvents. The mechanism of cyclization reaction by the natural orbital bond was studied.