Heterocumulenes Reactions with Organometallic Reagents: XV.* Quantum-Chemical Investigatiom of Skeleton Rearrangements of 2-Methyl-6-methoxy-3*H*-azepine Originating from Valence Tautomerism

V. A. Shagun, N. A. Nedolya, O. A. Tarasova, and O. G. Volostnykh

Faworsky Irkutsk Institute of Chemistry, Siberian Division, Russian Academy of Sciences,
Irkutsk, 664033 Russia
e-mail: nina@irioch.irk.ru

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Abstract—In the framework of quantum-chemical simulation (DFT) the structure was explored of six potentially probable tautomeric forms of 2-methyl-6-methoxy-3*H*-azepine and their relative thermodynamic stability was evaluated. In the tautomers obtained the preferred gradient channels are localized of [1,*n*]-H shifts capable of initiating their tautomerism. The most probable typical concerted reactions were analyzed of the formation of valence isomers, fused three-/six- and four-/five-membered carbo- and heterocycles, azabicyclo[4.1.0]hepta-2,4-dienes (azanorcaradienes) and azabicyclo[3.2.0]hepta-3,6-dienes respectively.

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