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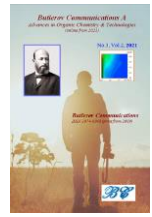

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Details of the formation mechanism 5-(pyridylmethylidenyl)-3-alkyl-2-thiohydantoines

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Keywords: 2-thio-5-(pyridylmethylidene)-3,5-dihydro-4H-imidazole-4-ones, 3-alkyl (aryl- or heteroaryl)-2-thioxo-imidazolidin-4-one, 3-R-2-sulfanylideneimidazolidin-4-one, 3-R-2-thioxoimidazolidin-4-one, *N*-alkyl(aryl) thiohydantoin, 2-thiohydantoin, 3-heteroaryl-2-thioxo-imidazolidin-4-one, quantum chemistry, 5-Z-structure, formation mechanism and dipole moments of 2-thio-5-(pyridylmethylidene)-3,5-dihydro-4H-imidazole-4-ones, free energy of formation.

Abstract

The features of the second stage of the reaction of the formation of a promising class of biologically active compounds 2-thio-5-(pyridylmethylidene)-3,5-dihydro-4H-imidazol-4-ones, proceeding through the formation of a reaction complex from reagents, a catalyst (KOH) and a solvation shell from solvent molecules, and the question have been considered and answered: “Is the formation of a 5-Z oriented product the same thermodynamically limited?" In order to find an answer to this question, the energies of formation of two stereoisomers and their rotational conformers 5-Z, as well as thioenol forms corresponding to compounds 5-Z, dipole moments and moments of inertia of rotational motion *J* along the *x*, *y*, *z* axes were calculated using quantum chemical methods. The analysis of the obtained calculated data on the energies of formation of alternative products, moments of inertia of rotational motion and their subsequent comparison with the experimental results shows that the formation of the Z-product is a symbate combination of both orientational interactions (dipole-dipole, hydrogen bonds) in the the transition state and the thermodynamic preference of the resulting product.

The data obtained also testify in favor of the need to attract, along with the traditional energies of formation of structures, the moments of inertia of the rotational motion J_x and J_z of individual supposed products, which, like the dipole moments, have a determining role on the

position of conformational equilibrium and stabilization of individual forms leading to the formation of the Z-5-(pyridylmethylideno)-structure. This confirms the earlier conclusion that the moments of inertia of the rotational motion J_x and J_z as characteristics of the rotational degree of freedom can act as numerical characteristics of the spatial structure of molecules.

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