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Research study of the reaction mechanism of triazoleoxide formation with the use of the density functional theory

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Abstract

Thermodynamic parameters of amination reaction in gaseous phase and in the solution have been analyzed using computations with the method of density functional and the use of full electron basic set 6-31G(d). Thermodynamic and kinetic reaction capacity for condensing dichlorojuglone with aniline has been shown. Transitive states, activation energies, as well as the rate and constants for the reaction of condensation have been computed.