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Investigation of the mechanism of amination reaction of dichloronaphtohynones on the base of density functional theory

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Abstract

The analysis of the thermodynamic parameters of the amination reaction in the gas phase and in solution based on calculations by density functional theory using all electron basis set 6-31G(d) in the software package GAUSSIAN'03 and TZ2P+ in The Amsterdam density functional program. It is shown the thermodynamic and kinetic reaction dichloronaphtohynones possibility with aniline. There are having been calculated the transition states, activation energies and the analysis of orbital interactions have carried out.