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Theoretical Evaluation of the Effect of Solvent on the Feasibility of the Reaction of 2-Chlorobenzimidazole With Four N,N′-Cyclic Azomethine Imines to Construct Polycyclic Benzimidazoles

Authors : Mohamed Abdoul-Hakim, A. Zeroual, H. Garmes

Abstract : In this work, we theoretically evaluated the reactivity of four 4-methyl-3-oxo-1,2-pyrazolidinium ylides with 2-Chlorobenzimidazole in MeOH in basic medium using DFT at the B3LYP/6-311+G(d,p) level. The analysis of the results shows that apart from its ability to retain its electrons, the deprotonated 2-Chlorobenzimidazole has a higher nucleophilic character. The reaction requires energy input to initiate the nucleophilic attack of the 2-Chlorobenzimidazole anion, and the inclusion of the solvent effect facilitates the formation of two regioisomers via an intramolecular vinyl nucleophilic substitution (SNVi). The transition states of this latter step are stabilized by charge transfer interactions σ(N-C) →σ*(C-Cl) for the more favorable regioisomer and n(N)→σ*(C-Cl) for the other regioisomer.

Keywords : benzonitrile N-oxide,DFT, intramolecular vinyl nucleophilic substitution (SNVi), 4-methyl-3-OXO-1, 2-pyrazolidinium ylides
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