Theoretical Evaluation of the Preparation of Polycyclic Benzimidazole Derivatives

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Abstract : In this work, the reaction of 2-chlorobenzimidazole with two distinct 1,3-dipoles such as benzonitrile N-oxide and an azomethine imine was carried out by DFT at the B3LYP/6-311+G(d, p) level to understand the effect of solvent (MeOH). The results show that MeOH has a significant effect on the evolution of the reaction. The charge transfer interactions $n(O) \rightarrow \sigma^*(C-Cl)$, $n(N) \rightarrow \sigma^*(C-Cl)$ and $\sigma(N-C) \rightarrow \sigma^*(C-Cl)$ stabilize the transition states in an intramolecular nucleophilic substitution (SNi) step of the imidoyl group. Finally, this study provides a theoretical basis for the design of different polycyclic benzimidazole.

Keywords: azomethine imine, benzonitrile N-oxide, DFT, intramolecular nucleophilic substitution (SNi), polycyclic benzimidazole

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