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# 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) → σ*(C-Cl), n(N)→σ*(C-Cl) and σ(N-C) →σ*(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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