

## Exploitation of the Solvent Effect and the Mechanism of the Cycloaddition Reaction Between 2-Chlorobenzimidazole and Benzonitrile N-Oxide

**Authors :** M. Abdoul-Hakim, A. Zeroual, H. Garmes

**Abstract :** 2-Chlorobenzimidazoles are amphoteric compounds and versatile intermediates for the construction of polycyclic heterocycles. In this theoretical study performed by DFT at the B3LYP/6-311+G(d,p) level, we showed that the most likely route to obtain benzimidazo[1,2-d]oxadiazole from the reaction of 2-Chlorobenzimidazole with benzonitrile N-oxide involves the presence of anionic species, a concerted mechanism is not possible. The inclusion of the effect of the polar protic solvent (MeOH) favors the course of the reaction. The key interactions causing bond formation and breakage were identified by ELF topological analysis.

**Keywords :** benzimidazo[1, 2-d]oxadiazole, benzonitrile N-oxide, DFT, ELF, polycyclic heterocycles

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