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Theoretical Evaluation of Oxirane and Aziridine Opening Regioselectivity, Solvent Effect, and Strength of Nucleophilic and Nucleofugal Groups for the Preparation of Benzimidazole-Fused 1,4-Benzoxazepine

Authors : M. Abdoul-Hakim,a. Zeroual,H. Garmes

Abstract : In a route for the preparation of 1,4-benzoxazepine fused to benzimidazole, the use of 2-(2-methoxyphenyl)-benzimidazole or styrene-derived N-tosylaziridine does not give the desired products. On this basis, we theoretically studied this reaction using DFT at the B3LYP/6-31+G(d) level. The analysis of the results shows a preferential nucleophilic attack of 2-(2-fluorophenyl)-benzimidazole on the terminal carbon atom of the Alkylepoxides and on the substituted carbon of N-tosylaziridine. Taking into account the solvent effect (DMF) makes the reactions spontaneous for the opening of epoxides and N-tosylaziridine and disfavors the intramolecularnucleophilic aromatic substitution reaction step of the products of the attack of 2-(2-methoxyphenyl)benzimidazole on an epoxide and those of the opening of N-tosylaziridine, which is consistent with the experiment.

Keywords : alkylepoxides, 4-benzoxazepine fused to benzimidazole imine, benzonitrile N-oxide, DFT, intramolecular nucleophilic aromatic substitution, N-tosyl aziridine
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