EFFECT OF LEWIS ACID CATALYSTS ON THE POSITIONAL SELECTIVITY OF THE ELECTROPHILIC AROMATIC SUBSTITUTION ON α-SUBSTITUTED THIOPHENES: A CONCEPTUAL DFT INVESTIGATION

Amina Ghomri , Sidi Mohamed Mekelleche

Abstract :

The α′/β regioselectivity of the electrophilic aromatic substitution of some thiophene α-substituted derivatives (R = CHO, COMe or CO2Me), catalyzed and not catalyzed by the Lewis acid, AlCl3, has been investigated by means of the local nucleophilicity index, recently proposed by Pérez et al. [J Mol Struct: Theochem895: 86, 2009]. The quantum chemistry calculations, carried out at the B3LYP/6-311G(d,p) level of theory, show that the α′-substitution is preferred in absence of the catalyst, while the β-substitution is more favored in the presence of the catalyst. The theoretical results, predicted using DFT-based reactivity indices, are in good agreement with the experimental outcomes.

Keywords : Electrophilic aromatic substitution; thiophene derivatives; DFT-based reactivity indices; local nucleophilicity indice; lewis acid catalysts.

Journal title / Revue : JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY, ISSN : 0219-6336, DOI: 10.1142/S0219633611006566, Issue : 4, Volume :10, pp. 435-445, AOUT 2011.