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

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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: Theocm895: 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.