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Kinetics, Mechanism and Novel Methods Of Esterification

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Abstract: *The susceptibility of the carbonyl group towards nucleophilic attack affords the construction of various organic compounds. Thus, investigations of carbonyl activation applying greener methodologies are highly important. In the present work, among the investigated N-halo compounds, N-fluorobenzenesulfonimide (NFSi) has been found as an efficient and selective catalyst in the reaction of direct esterification of aryl and alkyl carboxylic acids supported by microwave (MW) irradiation. The comprehensive esterification of different benzoic acids and mono-, di- and tri-carboxy alkyl derivatives was performed, whereby significant reaction time reductions were achieved. The presented method used NFSi as an easily manipulatable, non-metal, water- and air-tolerant catalyst, allowing simple synthetic and isolation procedures and energy saving, compared to conventional methodologies. Importantly, in contrast to esterification under thermal conditions, where N-halo compounds behave as pre-catalysts, in the MW-supported protocol, a distinct reaction mechanism has been proposed that assumes NFSi as a sustainable catalyst. Moreover, a scale-up of the industrially important derivative was performed.*
Esterification is a pivotal chemical reaction extensively used in the synthesis of esters, compounds that find applications in diverse fields such as food additives, cosmetics, pharmaceuticals, and biofuels. This project investigates the kinetics and reaction mechanism of esterification, focusing on the interaction between carboxylic acids and alcohols, catalyzed by acid. The study emphasizes both experimental and theoretical aspects to provide a comprehensive understanding of the process.

Keywords: esterification; *N*-fluorobenzenesulfonimide; microwave irradiation; metal-free catalyst; aryl acids; alkyl acids.

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