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High regioselective process for the production of important industrial intermediates in high yields

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The products from aromatic nitration are very important intermediates for the production of many industrial products such as pharmaceuticals, dyes, polymers, perfumes, and fertilizers. For example, 2,4 dinitrotoluene can be used for the production of toluene diisocyanate (TDI) and toluenediamine that can be used to produce polyurethane. Polyurethane is widely used in varnish, wheels, furniture and has many other applications.

We have investigated the dinitration of toluene over zeolite under various reaction conditions with the aim to produce 2,4-DNT selectively and in high yield. The best result obtained under produce 2,4-DNT in 90%. Therefore, in an attempt to push the reaction to completion, various acid anhydrides (e.g. anhydrides with different carbon chain length, halogenated acetic anhydrides) were used along with various quantities of zeolites and reagents.

It was found that chloroacetic anhydride over Hβ produced 2,4-dinitrotoluene in 98% yield in which 2,4-:2,6-DNT was 49:1. Also, propionic anhydride under similar reaction conditions produced 2,4-DNT in 98% but in excellent selectivity (2,4-:2,6-DNT=123:1). This result is simply the highest for direct dinitration of toluene ever recorded. In contrast to traditional method, the system containing propionic anhydride, nitric acid, zeolite Hβ gave excellent yield of 2,4-dinitroyoluene with excellent selectivity and the only by-product produced during the process was the propionic acid which can be recycled easily. Also, the zeolite can easily remove from the reaction mixture by simple filtration, activated and reused to give good results for several times. The system was applied successfully to various mono-substituted benzenes (e.g alkyl and akyloxybenzene).

Biography

Mohammad Alotaibi has completed his Ph.D. at Cardiff University. His research involves development of novel organic synthetic methods, especially ones that are “greener” than traditional methods. Also, has great interest towards synthesis of compounds with interesting properties. Particular current research projects involve use of zeolites and solid-supported reagents as catalysts to gain regioselectivity in organic reactions. Active collaborations exist with Professor Keith Smith, Cardiff University, United Kingdom and Professor Gamal A. El-Hiti, King Saud University, Saudi Arabia.

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