

# ALKYLATION OF PHENOLS USING IONIC LIQUID CATALYSTS

by

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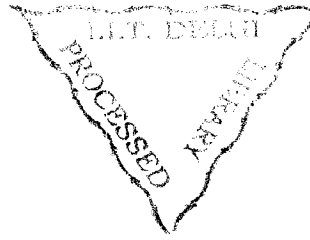
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## CERTIFICATE

This is to certify that the report titled “**Alkylation of phenols using ionic liquid catalysts**” is a bonafide record of the project work carried out by **P. Elavarasan** (2007CHZ8214) under my supervision and guidance, in fulfillment of the requirements for the award of the degree of **Doctor of Philosophy**. Further, to the best of my knowledge this has not been submitted to any other University or Institute for the award of any Degree or Diploma.

Date : 7/1/2011



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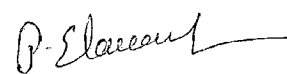
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## ABSTRACT

Alkylation of aromatics is of immense importance to the chemical and petrochemical industry. Alkylation processes were traditionally conducted using Friedel-Crafts catalysts. In recent years these are being replaced by more economical, energy saving and environmentally benign catalysts. Also, the use of alcohols as alkylating agents is being researched the world over due to the inherent problems of transportation, handling and unavailability of alkenes. The present work is focused on investigating the alkylation reaction of phenol and *p*-cresol with *tert*-butyl alcohol to produce 2, 4-*tert*-di-butylphenol (2, 4-DTBP) and 2-*tert*-butyl-*p*-cresol (TBC), 2,6-di-*tert*-butyl-*p*-cresol (DTBC) respectively. An attempt is made to develop novel Bronsted acidic ionic liquid catalyst system that could be used efficiently in this reaction.

The ionic liquids and supported ionic liquid catalyst were prepared in the laboratory and characterized using NMR, TG-DTA, SEM and FTIR. A statistical design of experiments was used to predict the effect of various process variables on the phenols conversion and desired product selectivities. Experimental kinetic investigations were conducted in a batch autoclave and the optimum temperature, reaction time, reactant mole ratio and reactant to catalyst ratio are reported. The catalysts were found to be completely recoverable and recyclable.

A reaction mechanism was proposed based on the product distribution obtained from experimental investigations. Semi-empirical computations were used to model this reaction system and further assess the reaction pathway and mechanism. Based on the proposed reaction mechanism, kinetic models were developed and the kinetic parameters were estimated using non-linear Marquadt's routine.

*Key words:* alkylation, *tert*-butylation, phenol, *p*-cresol, 2, 4-*tert*-di-butylphenol, 2-*tert*-butyl-*p*-cresol, 2,6-di-*tert*-butyl-*p*-cresol, ionic liquid, supported ionic liquid, kinetics.

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