A STUDY OF THE REGIOSELECTIVITY IN THE ZEOLITE-ASSISTED NITRATION OF TOLUENE

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A Thesis Submitted to the
University of North Carolina at Wilmington in Partial Fulfillment
Of the Requirements for the Degree of
Master of Science

Department of Chemistry

University of North Carolina at Wilmington

2003

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ABSTRACT

Nitration of toluene has been an important industrial process for many years. The conventional method is effective in nitrating toluene, but it produces an ortho:meta:para (o:m:p) ratio of approximately 57:4:39, respectively. There has been considerable effort studying the potential for various zeolites to influence regioselectivity towards the *para*-isomer, which is the most desirable isomer. By introducing zeolites into the process, the regioselectivity can be directed with the proper selection of the pore size of the zeolite used. The use of the zeolite catalysts improved the regioselectivity of the reaction and has produced the *para*-isomer as high as 80%.

It has been reported that the increase in regioselectivity is related to the silica/alumina ratio (SAR) of the zeolites used. This is somewhat unexpected based upon size selective reactions in other zeolite systems. Our investigations of the zeolite assisted reactions led to the conclusion that the increase in the regioselectivity of these reactions did not depend on the SAR, as previously reported, but is due to the pore size of the zeolite. The improved zeolite reaction produced an isomeric distribution of 18% ortho-, 0.52% meta-, and 82% para-mononitrotoluene with more readily available zeolites.

While investigating the regioselective zeolite reaction, a side product was noted that had not previously been reported with respect to this reaction. This side product was considered a contaminant initially and its production was minimized during the reaction. The contaminant was identified as phenylnitromethane, PNM and it was determined that its production was significantly different from the nitrotoluene in that a radical reaction was responsible instead of an aromatic substitution. After identification, it was decided

to take advantage of this side reaction to produce the PNM, as the reported methods were difficult and/or time-consuming syntheses.

The zeolite method for producing the PNM was investigated and yielded 3.00g of phenylnitromethane (94% purity by GC).

ACKNOWLEDGEMENTS

I would like to thank Dr. John Tyrell for all of his help and support throughout this project. Without his patience and humor, these past months would have been a far less enjoyable journey.

To Heather McCreery, I give heartfelt thanks for all of the moral support and for being there to listen to the gripes and groans of a frustrated graduate student (whom I believe she once was).

My thanks to the rest of the faculty of the Chemistry Department for loaning materials, time, and experience to that same frustrated graduate student.

To Ned Hill who kept the computers, printers and various other gizmos and gadgets in the lab running when they should have been consigned to oblivion long ago, many thanks.

To Miss Shearon and Miss Libbie for all their help and for putting up with the seemingly unending stream of questions about when, where, and how to do just about everything.

Finally, I must thank Jennifer Jones for putting up with me through the good and the bad and for always telling it like it is.

DEDICATION

I would like to dedicate this thesis to my family for without their guidance and support this would not have been possible. And a special dedication of the knowledge represented in this work to my nephews, Chandler and Gannon, who represent the bright possibilities of the future.

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