EXPERIMENT 5: DATA SHEET

Electrophilic Aromatic Substitution: A Friedel-Crafts Acylation Reaction

DUE: The week of March 19, 2007 – during your lab. This will allow time to analyze the NMR and IR spectra.

Name:	
Lab Section:	
Demonstrator:	

UNKNOWN Aromatic= A, B, C, or D

After determining the identity of your unknown aromatic draw the reaction equation showing the structures of starting material and possible products. Be sure to name the compounds using IUPAC rules:

Calculate your yield:	
Acetyl chloride: Molecular Weight =	
Volume used =	
Grams used =	
Moles used =	
Unknown Aromatic (): Molecular	Weight =
Volume used =	Grams used =
Moles used =	
Limiting reagent:	
Product:	
Molecular Weight =	
Moles Expected =	
Grams expected =	(theoretical yield)
Mass of round bottom flask and stoppe	er =
Mass of round bottom flask, stopper ar	
Net Mass of products obtained =	<u></u>
Percentage Yield: =	-

Show calculations on reverse.

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 Discuss briefly possible reasons (other than experimental error) for a less than 100% yield. (if your yield was over 100% discuss possible reasons). 	
 Describe the appearance of your product (solid, oil, liquid, viscous or not, colour etc. If 	
you were able to get a melting point, record the value here and discuss. (Is it sharp or broad? Does the m.p. match that expected for what you think the major product is based on your analys below? If your product is a liquid how would you purify it (you know at least two ways)?	S
 Draw a representation of your TLC plate. Determine R_f values of your product(s) and 	
unknown aromatic and comment on purity of your reaction product.	

Analysis of NMR Spectrum of Product:

Attach your NMR spectra to this Data Sheet. Assign a structure of your product by completely analyzing your ¹H and ¹³C NMR spectra. In some cases it may be possible to see more than one of the disubstituted benzene products. Be sure to integrate all peaks and assign a relative proportion of the products.

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Analysis of Infrared Spectrum:

Attach and analyze the IR spectrum of your products, assigning appropriate peaks. Compare and comment on it compared to the IR spectrum of the starting material (provided in the laboratory). Also use Table 1 in experiment 4 to try to determine (confirm) the substitution pattern of your product (*ortho, meta or para*).

Draw a $\underline{complete\ mechanism}$ of the reaction on your unknown aromatic with acetyl chloride + AlCl₃ accounting for any regiochemistry.