Chem318 Electrophilic Aromatic Substitution 02/06/07 Bromination of Toluene

The electron-rich π -systems of aromatic rings make them susceptible to electrophilic aromatic substitution. In such cases, electrophiles are electron deficient species that carry either a positive charge or a partial positive charge.





Electrophilic aromatic substitution.

In halogenation reactions, benzene (toluene) does not react with bromine or chlorine by themselves. However, the presence of a Lewis acid such as FeBr₃, AlCl₃ or FeCl₃ can serve to catalyze the reaction. (Fluorine is much more reactive than either chlorine or bromine and iodine is much less reactive)





In the case of toluene you have a methyl substitutent already on the ring. Therefore the bromine must add at one of the other positions. This would provide for *ortho* (o), *meta* (m) and *para* (p) substitution products.



Bromination of toluene and possible substitution products.

As seen in the above figure, toluene has five hydrogen atoms (sites for bormination), two are ortho to the methyl group, two are meta and the fifth is para. Assuming that all positions were equally favored, we would expect a product mixture where 40% of the product was ortho, 40% meta and 20% para (or a product ratio of 2:2:1, o/m/p).

However, this may not be the case. It is possible that not all of these products are equally favored. Therefore, we may not observe this ideal ratio of isomers. We will evaluate the isomeric distribution of products based on IR spectra. Each isomer has a characteristic absorption band between 700 and 810 cm⁻¹ (o-bromotoluene 747 cm⁻¹, m-bromotoluene 770 cm⁻¹ and p-bromotoluene 801 cm⁻¹). In absorption spectra, the peak area for each isomer is proportional to its relative abundance.



Peak Area = h x w_{1/2}