Answer on Question #39828-Chemistry-Organic Chemistry

Question

Describe why SEAr reactions of toluene lead to ortho and para products while SEAr reactions of benzaldehyde lead to only meta-products. Use convincing mechanistic arguments and show all important structures or resonance forms to support your explanations.

Answer

In electriphilic substitution reactions into benzene ring (SEAr) an electrophil attacks positions, which are more negatively charged.

In case of toluene +M effect takes place, namely σ - π hyperconjugation of the three C–H bonds of the methyl group with π -electrons of benzene ring, which makes the ring partially negatively charged. Distribution of this partial charge results in ortho- and para-positions to gain more electron density:

That is why an electrophil (E⁺) attacks ortho- and para-positions and does not attack meta-positions, resulting in ortho- and para-products:

The positively charged intermediate σ -complexes are stabilized by **+M** effect.

In case of benzaldehyde the carbonyl group proves -M effect (π - π conjugation) due to the high electronegativity of oxygen atom. As a result electron density is drawn from the benzene ring making it partially positively charged. Distribution of this partial charge results in ortho- and para-positions to become most positive:

That is why an electrophil can not attack ortho- and para-positions. Metha positions are much less positive (almost neutral) so an electrophil attacks only these positions resulting in meta-products:

The positively charged intermediate $\sigma\text{-complex}$ is destabilized by $\textbf{-}\textbf{\textit{M}}$ effect.