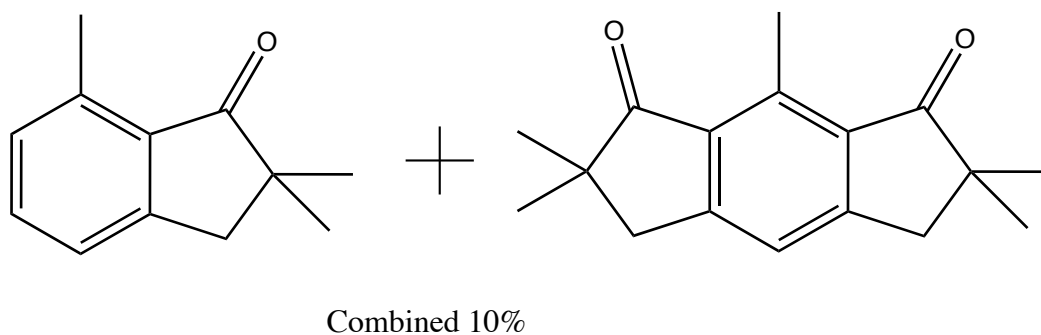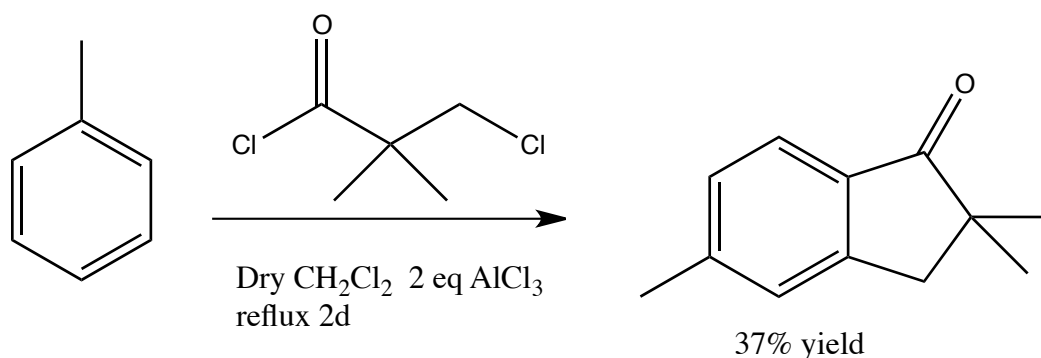This acylation/alkylation reaction proceeded as expected. T-butyl group is used to prevent HCl elimination after acylation. The conditions shown for both reactions are the conditions that yielded the best results.

Combined 10%

This reaction did not yield expected results. First tried the reaction under the same conditions. 15% yield obtained. Next, the order of addition was changed, cooled solution initially (acetone/CO$_2$), dry everything, reagents confirmed pure by NMR, toluene as solvent, increase reaction time to 2 days etc.

The temperature was also increased to reflux in dcm and toluene (excess), and the best results obtained are displayed in the picture above (yield determined by crude NMR with spike). Because of the methyl group toluene should be a better nucleophile; Marcus Theory states that toluene has a lower ΔG energy barrier (faster) compared to benzene as a nucleophile. The ratio of para/ortho addition makes sense because of steric crowding.

An additional unknown solid (expected products are liquid), shown by high-res MS, to be a 1:1 addition chlorine containing compound, was about 30% yield. Me+2 grad students with 2D-NMR couldn't figure out the structure within the time allotted. I think it is plausible radical formation causing a side reaction or $AlCl_3$ interacting with the methyl group; e.g., $AlCl_3$ has been shown to isomerize xylene.

My conclusion: because the ortho and meta states have higher ΔG, thus lower representation in the final equilibrium (toluene rxn). Benzene can probabilistically interact more with the reagent; therefore, creating a higher chance that the reaction ends up at the desired product at equilibrium. The unknown solid came from the reaction length (side reaction of radical, methyl-$AlCl_3$ reaction, or acid catalyzed side rxn). What do you think is right/wrong about the logic of this paragraph?