Stephanie Rugg
Organic Lab Thursday afternoon

Friedel-Crafts Mechanism:
The Theory Underlying The Synthesis of 1,4-Ditertbutylbenzene

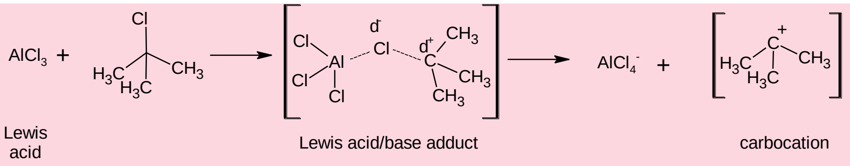
Commented [RSC1]: Detailed Title: What are you studying?

Commented [RSC2]: Turn this in as a separate document.

Theory

Commented [RSC3]: ***Theory (1-2 pages)*** *should be focused on the mechanism governing the reaction run. Pictures and diagrams (e.g. activated complexes and reaction coordinate diagrams are smiled on).Here, you attempt to sound like the text. Be precise and correct in your language. Follow rubric hints. Either draw very neatly or use Chemsketch for your structures.*

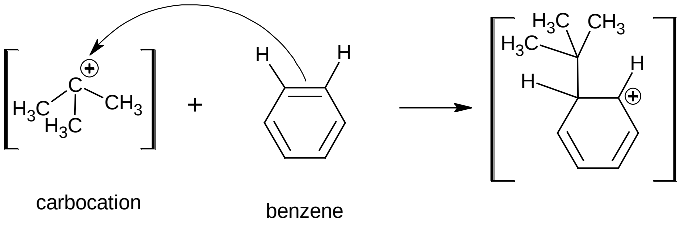
Friedel-Crafts substitution reactions generally involve the use of the powerful Lewis acid, such as aluminum chloride ($AlCl_3$), to generate a positively charged electrophile, which is then substituted into the targeted substrate. In the current experiment, the reaction generating the electrophile is described by reaction **1:**



(1)

Commented [RSC4]: Label your structures so you can refer to them in the text. The number on the right is the equation or reaction number.

The other substrate in the pot is the benzene ring, which is very electron rich. This benzene will attack the electrophile, the positive carbocation. Electrons are removed from the adjacent carbon in the ring, giving it a formal positive charge (2).



(2)

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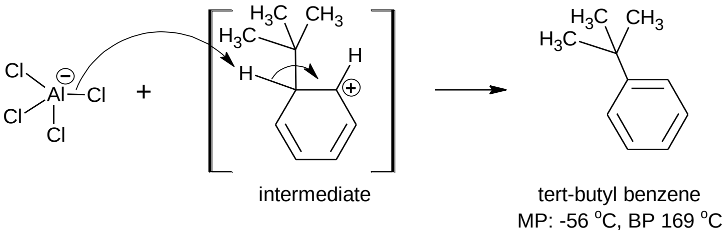
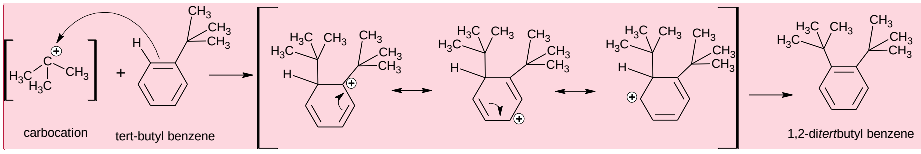
Finally, the benzene ring needs to be re-aromatized. The extra chlorine on the aluminum takes the hydrogen (from the carbon with the new tert butyl group), and those electrons from the C-H bond go to make the double bond, canceling out the formal positive charge on the adjacent carbon to make tert-butyl benzene (3).

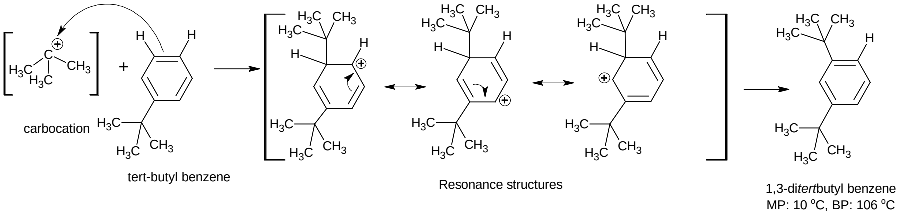


(3)

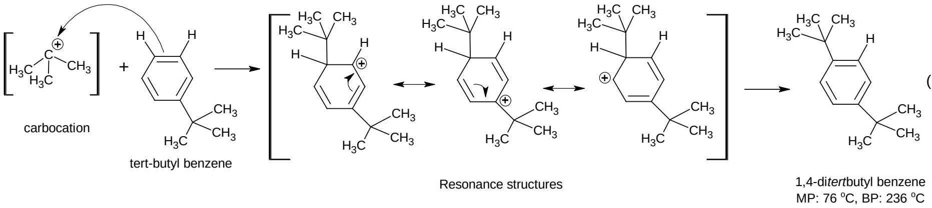
The reaction does not cease with the formation of a monoalkylated ring. Another tert-butyl group can be added to the benzene ring, with the ring attacking the electrophile. Because the ring already contains a substituent, it can add ortho (4), meta (5), or para (6) with each having multiple resonance structures. Rearomatization occurs as in step 3.



(4)



(5)



(6)

Commented [RSC5]: Show all possible outcomes, and explain why your product will prevail.

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The resonance structures have a carbocation in various positions on the benzene ring. For the resonance structures when adding ortho and para, the carbocation ends up at the base of the existing tert-butyl group, where as when adding meta the carbocation does not end up at this position. The existing tert-butyl group is electron donating (through inductive effect), therefore it stabilizes the positive charge. Therefore, the ortho and para structures are favored over the meta.

Between the ortho and para structures, sterics takes over. The tert-butyl group is “bulky”, and therefore the two groups would prefer to be further apart from each other, therefore the para product is the predicted product.