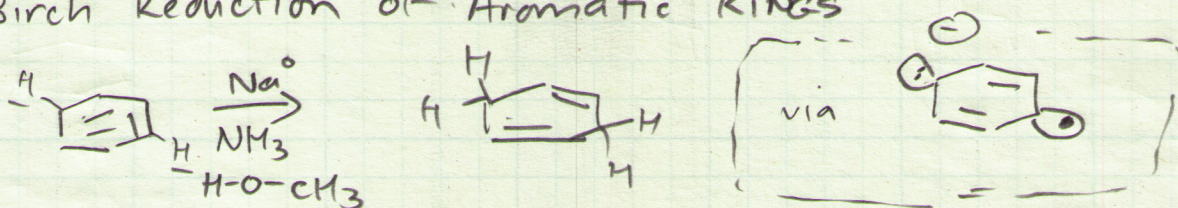


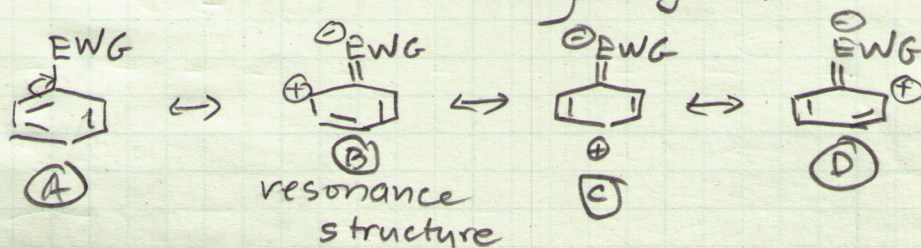
Birch Reduction of Aromatic Rings



See NOTES from 03-14-2025

Substituent effects on Birch Regioselectivity

EWG: electron withdrawing group
 EDG: " " donating group

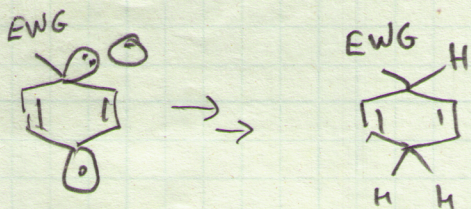


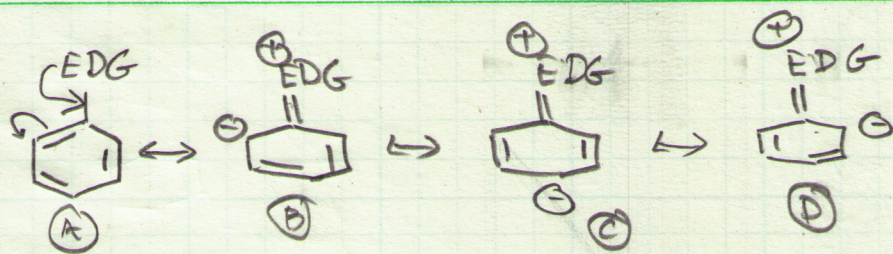
Also notice inductive electron withdrawal at the ipso carbon of the aromatic ring; i.e., the carbon attached to the substituent



ipso C. has δ^+ charge that can support a \ominus charge or Radical
 the δ^+ is a direct consequence of the dipole created by the EWG!

\therefore a Birch Reductⁿ intermediate is supported by a combination of the dipole and resonance structure C above





ipso C has δ^- charge in this scenario and thus cannot support a $(-)$ charge or radical as well. This direct induction effect is creates Birch reductⁿ selectivity directing the anion and radical.



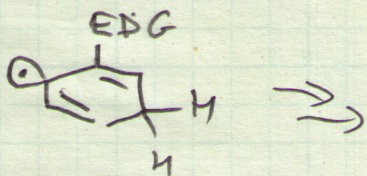
radical here

None of the resonance str above has δ^- here so $(-)$ charge is supported and commits the regioisomerism to this position.

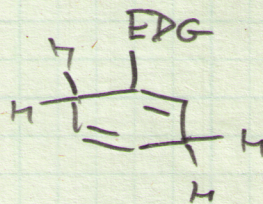
" - "

while res str (B) place δ^- here a radical can be supported; no $(-)$ formal charge is present on the C!

once this commits



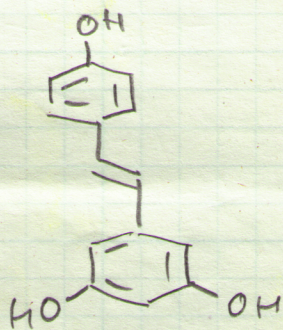
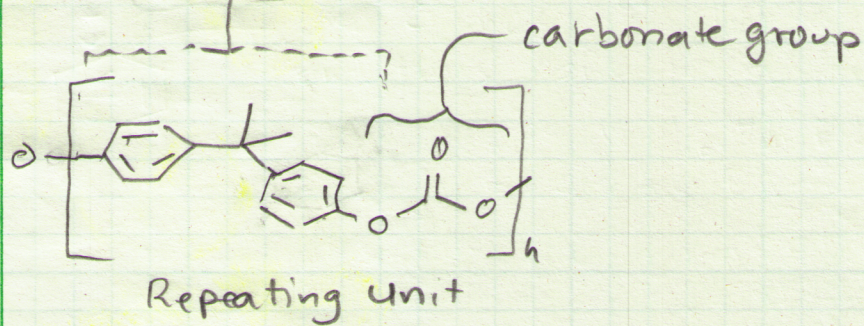
then this results



Phenols

Polycarbonate Filament in 3D Printing.

²
bisphenol : two "phenols"

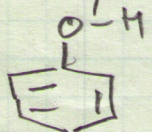


Resveratrol

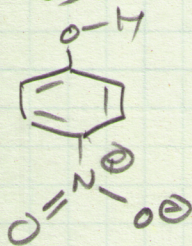
found in Wines

(cancer chemo preventative)
(reduces heart disease)

Acidity of Phenol(s)

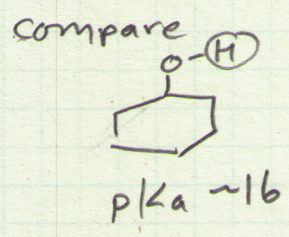
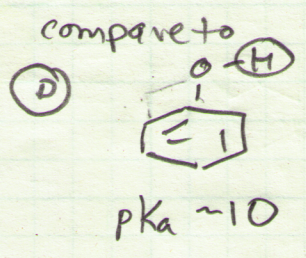
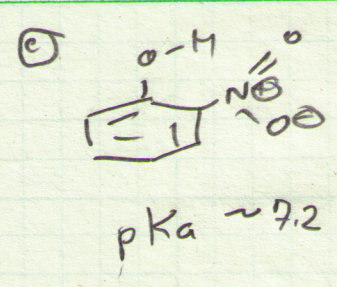
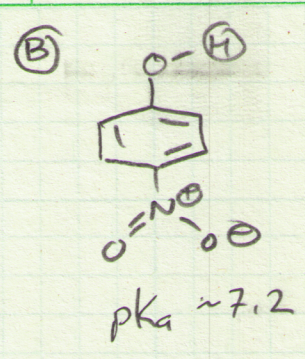
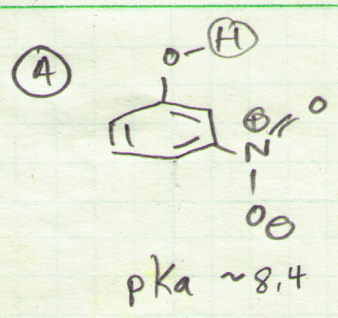


pKa 10



pKa ~7.4

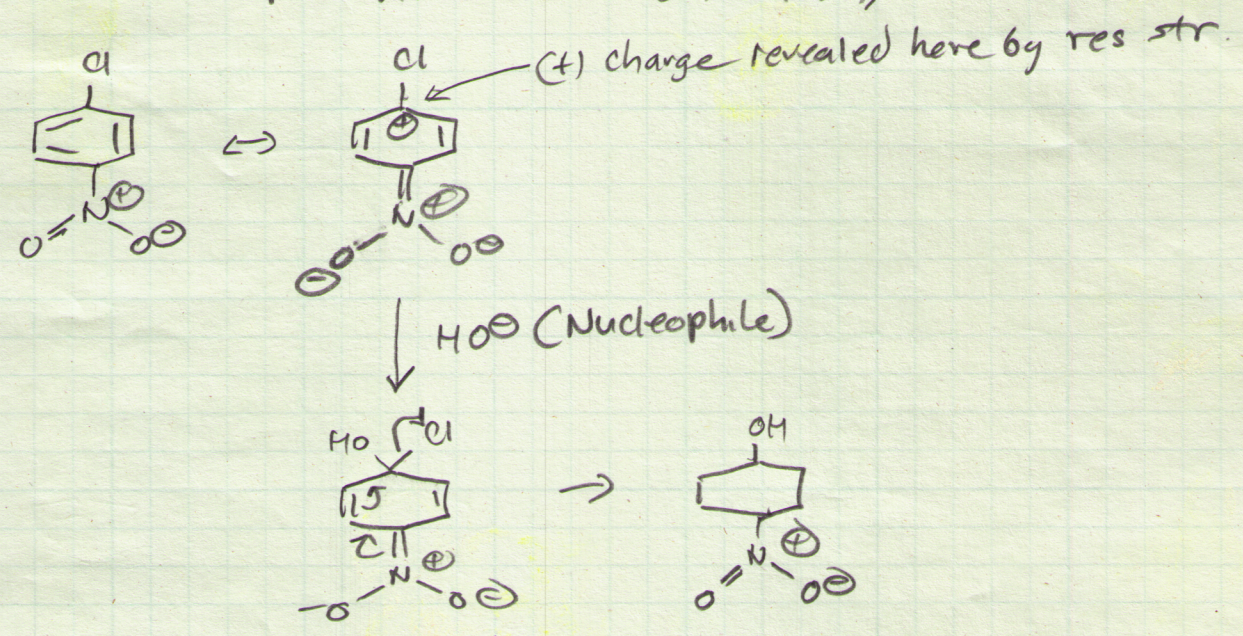
why?



why is the pKa of (A) > B/C but < (D)?
 Resonance Induction

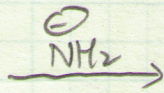
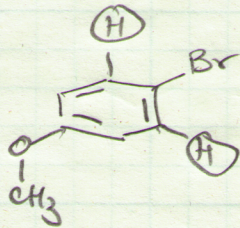
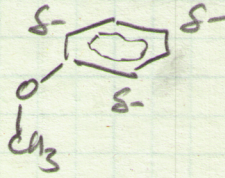
Preparation of Phenols

NAS (Nucleophilic Aromatic Substitution)



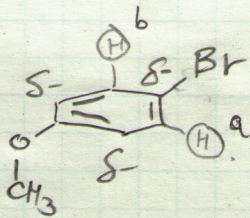
Revisit

Resonance Hybrid

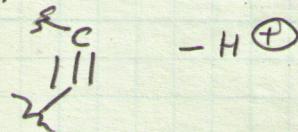


These "Elimination Rxns" (stepwise) are affected by the nature of the substituent that is strongly EW or ED (electron withdrawing or electron donating)

EDG

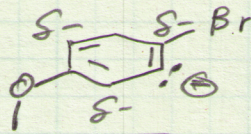


Technically the "Br Lig." Br^- can leave first to leave a δ^+ behind, which is then quenched by removal of the adjacent H^+



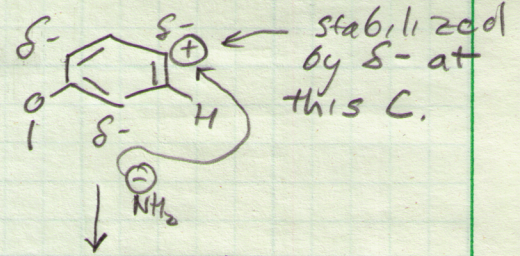
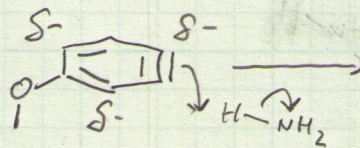
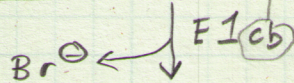
but let's evaluate the rxns in terms of H^+ removal to simplify the evaluation.

Remove H^a : yields

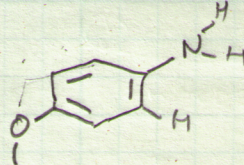
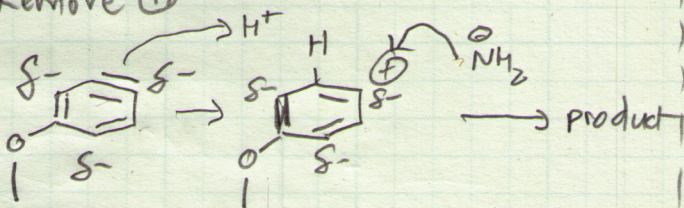


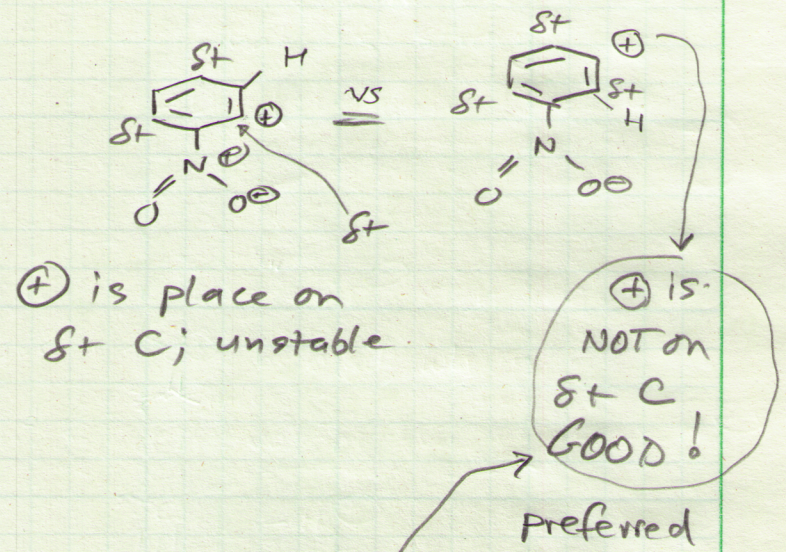
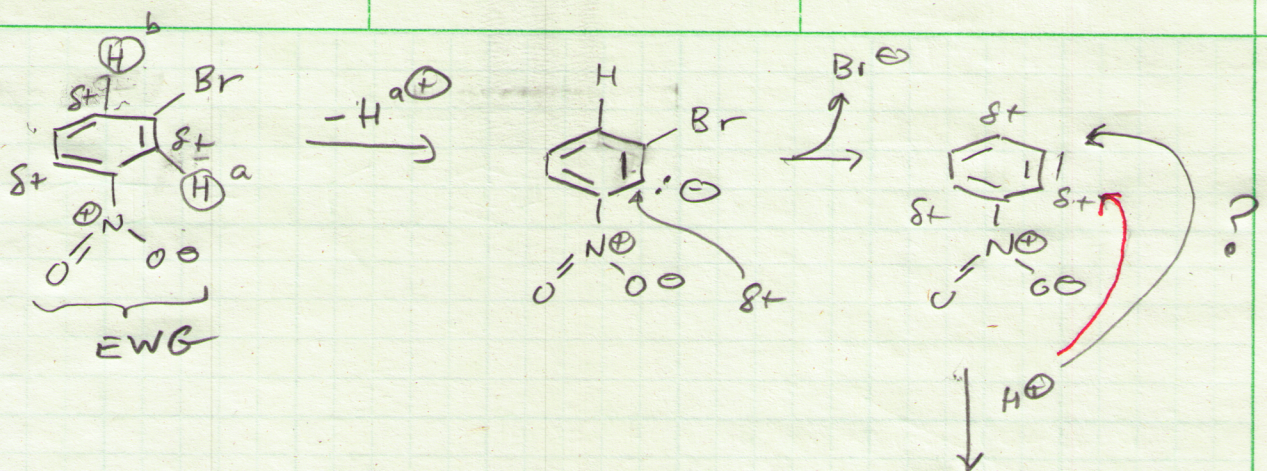
NOTE: Formation of this (-) is favorable as it does not form on a δ^- -C.

conjugate base

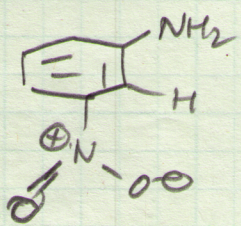


Remove H^b

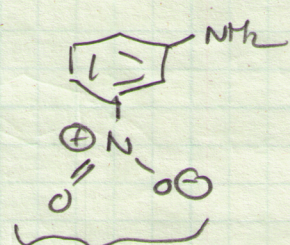
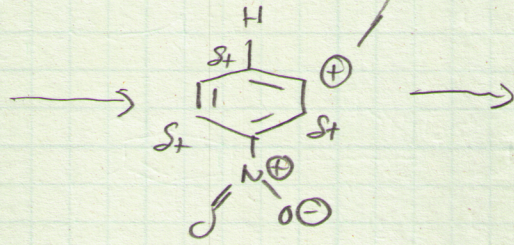
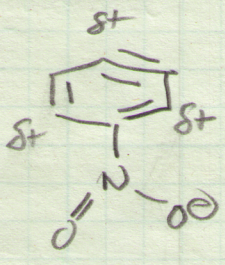




MAJOR PRODUCT IS



compare



same as above