

10/19/11

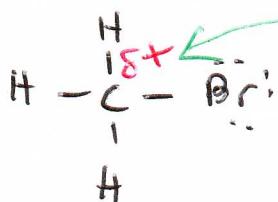
#1



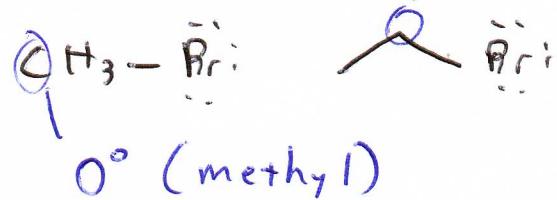
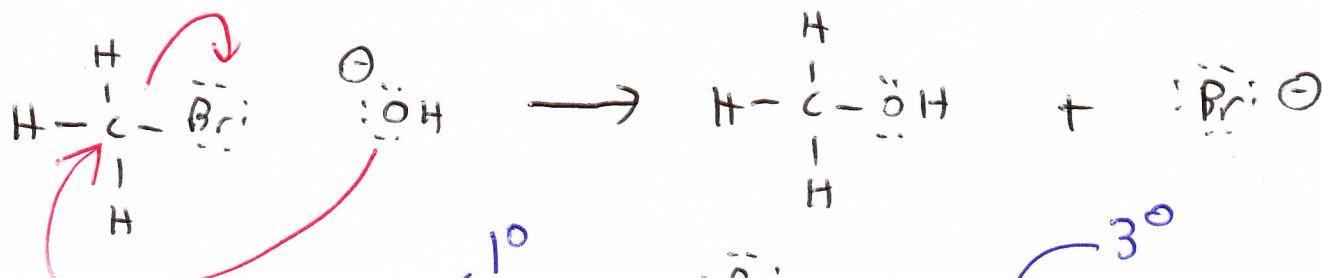
bromomethane  
methyl bromide

haloalkane  
alkyl halide

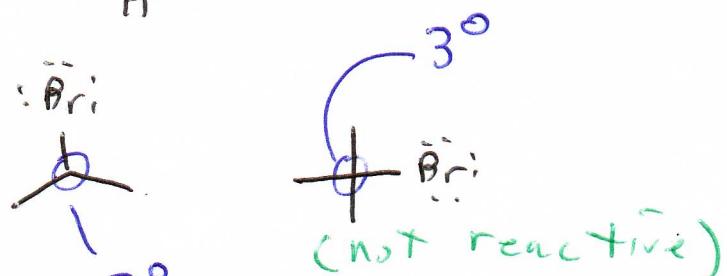
systematic  
common



$\text{O}^-$  electrophile - seeking  $\ominus$  charge  
 $\text{:}\ddot{\text{O}}\text{H}$  nucleophile - seeking  $\oplus$  charge

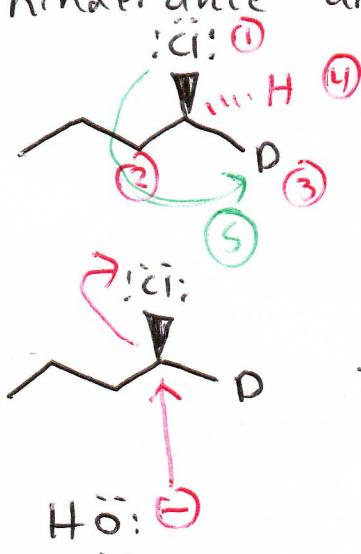


$0^\circ$  (methyl)



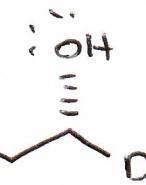
Increasing reaction rate

Methyl and primary alkyl halides react more quickly by this mechanism than  $2^\circ$  or  $3^\circ$  alkyl halides because there is less steric hindrance around the reaction site.



(S)-1-chloro-1-deuterobutane

Inversion of configuration - geometry  
at a stereocenter is inverted during a rxn



R2 regiochemistry - refers to whether a rxn occurs at only one site or @ multiple sites

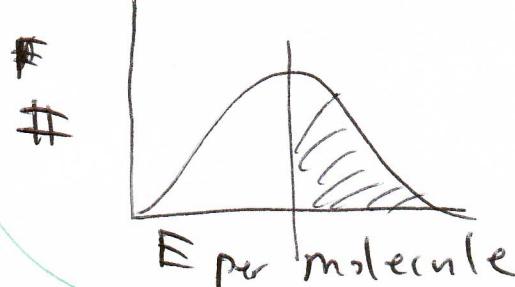
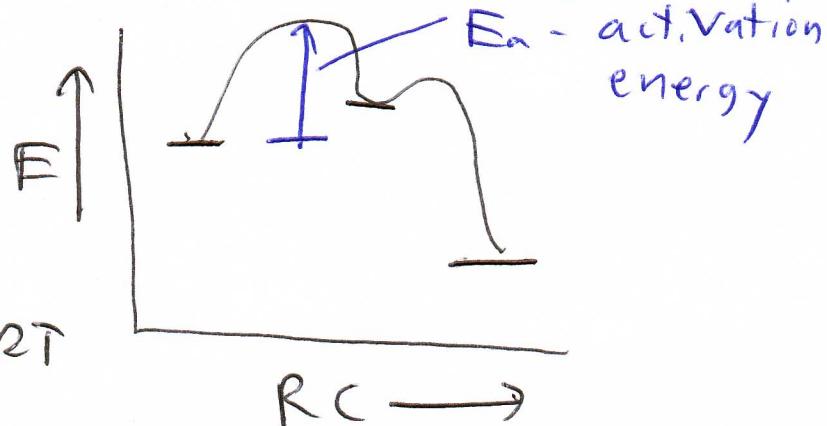
## B. molecular nucleophilic substitution ( $S_N2$ )

$$R = k[ \text{I} ][ \text{E} ]$$

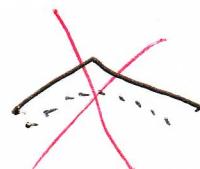
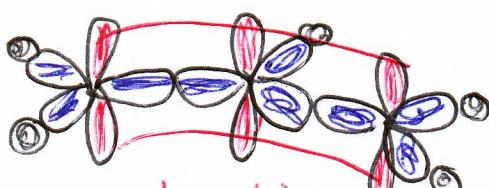
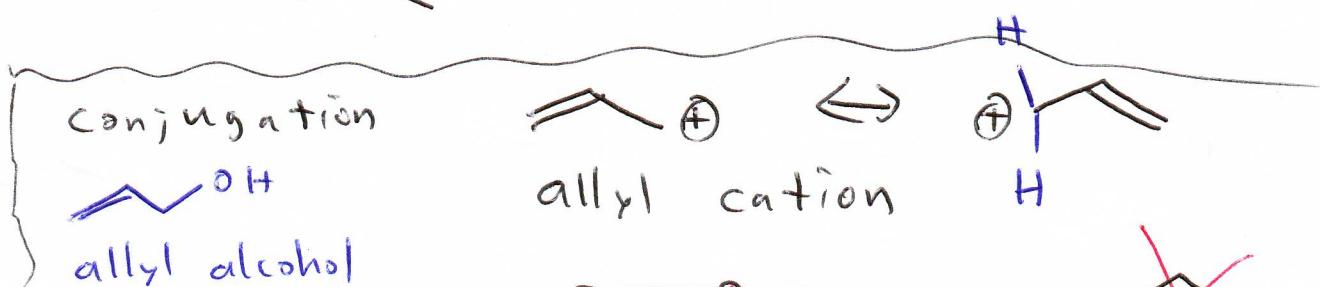
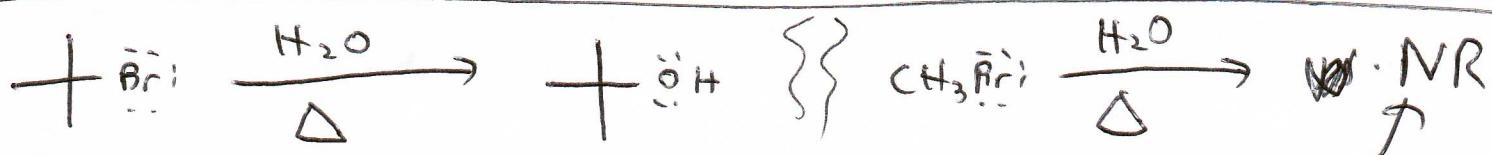
RLS - rate-limiting step

- individual step with the largest activation energy

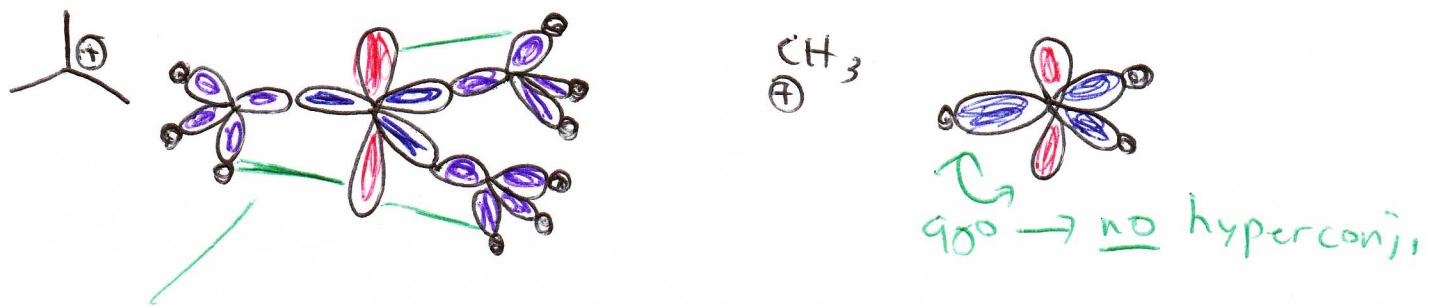
$$k = A e^{-\frac{E_a}{RT}}$$



Both the nucleophile and the substrate react simultaneously in the RLS.



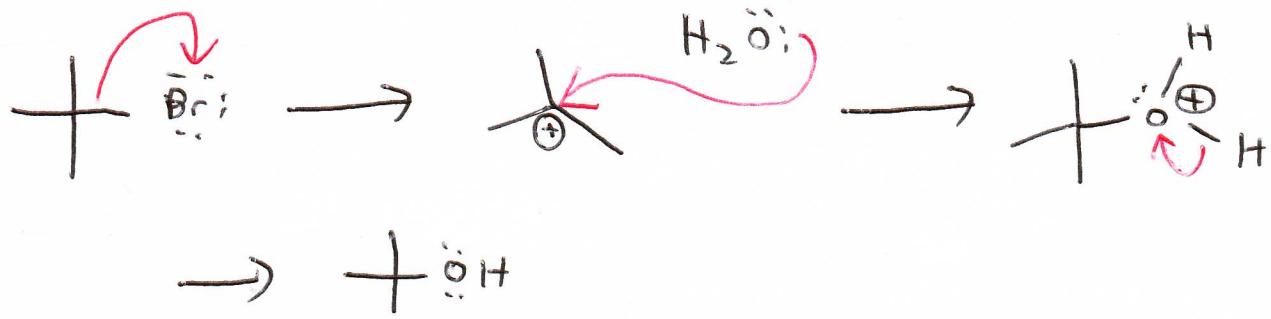
conjugation - a bonding interaction that involves more than two atoms.



hyperconjugation — a non-bonding orbital interaction

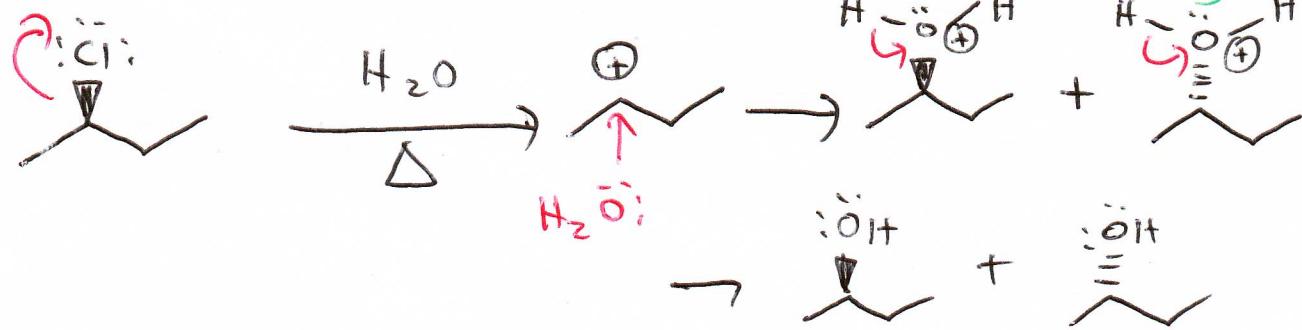


In this type of rxn,  $3^\circ$  alkyl halides are much more reactive than methyl or  $1^\circ$  alkyl halides because the carbocation formed during the reaction is more stable



### Unimolecular Nucleophilic Substitution (S<sub>N</sub>1)

Only one molecule is involved in the RLS (formation of the carbocation)



#4

