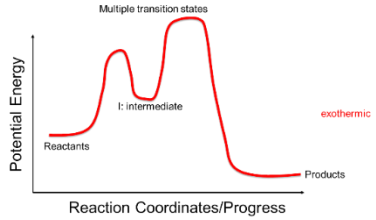
In class review (November 21 and 22)

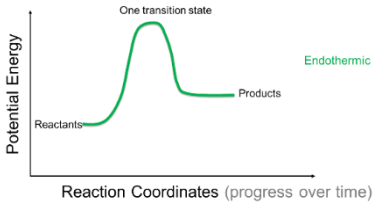
Major Concepts Covered from Videos 30-33:

Reaction pathways

Step-wise reaction

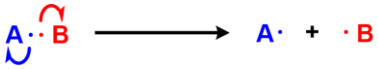


Concerted (one-step) reaction

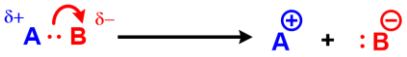


Bond cleavage and formation

Homolysis

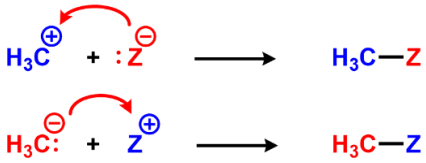


Heterolysis



Bond formation

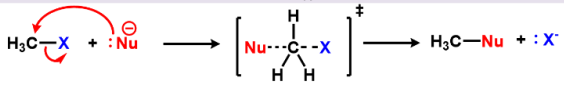
NUCLEOPHILE – electron rich species (seeks a positive center)
ELECTROPHILE – electron deficient species (seeks e⁻ to fill octet)



Nucleophilic substitution mechanisms

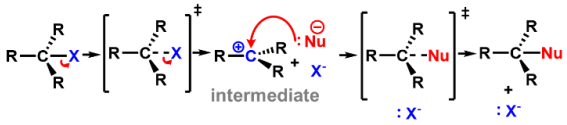
Two nucleophilic substitution (SN) reaction mechanisms

A: The nucleophilic attack and the leaving group departure occurs in one-step: Concerted: S_N2



transition state

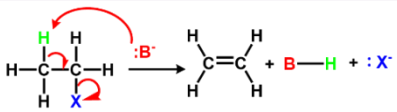
B: Reactants converted to products via more than one step: S_N1
Step 1: Heterolytic **cleavage** of C-X bond – carbocation formed
Step 2: Then nucleophile attacks the electrophile



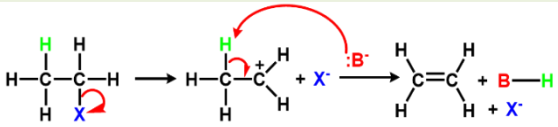
Elimination mechanisms

Two elimination (E) reaction mechanisms

1: Bond breaking and bond formation occur one-step: E2

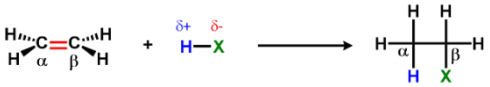


2: Reactants converted to products via more than one step: E1
Step 1: Heterolytic cleavage of C-X bond – carbocation formed
Step 2: Nucleophile attacks the electrophile

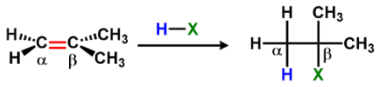


Electrophilic addition to alkenes

ELECTROPHILE – hydrogen of H-X (or other δ+ of x-X reagent)
NUCLEOPHILE – "attacking" π bond



Markovnikov's rule: hydrogen adds to the carbon in the double bond that has more hydrogen atoms, and **the halogen adds to the carbon with fewer hydrogen atoms**



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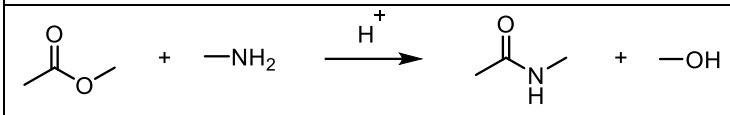
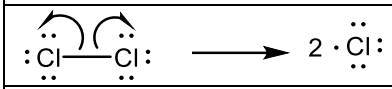
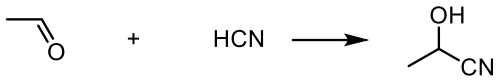
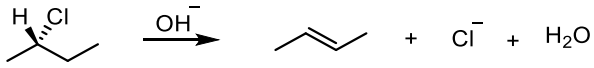
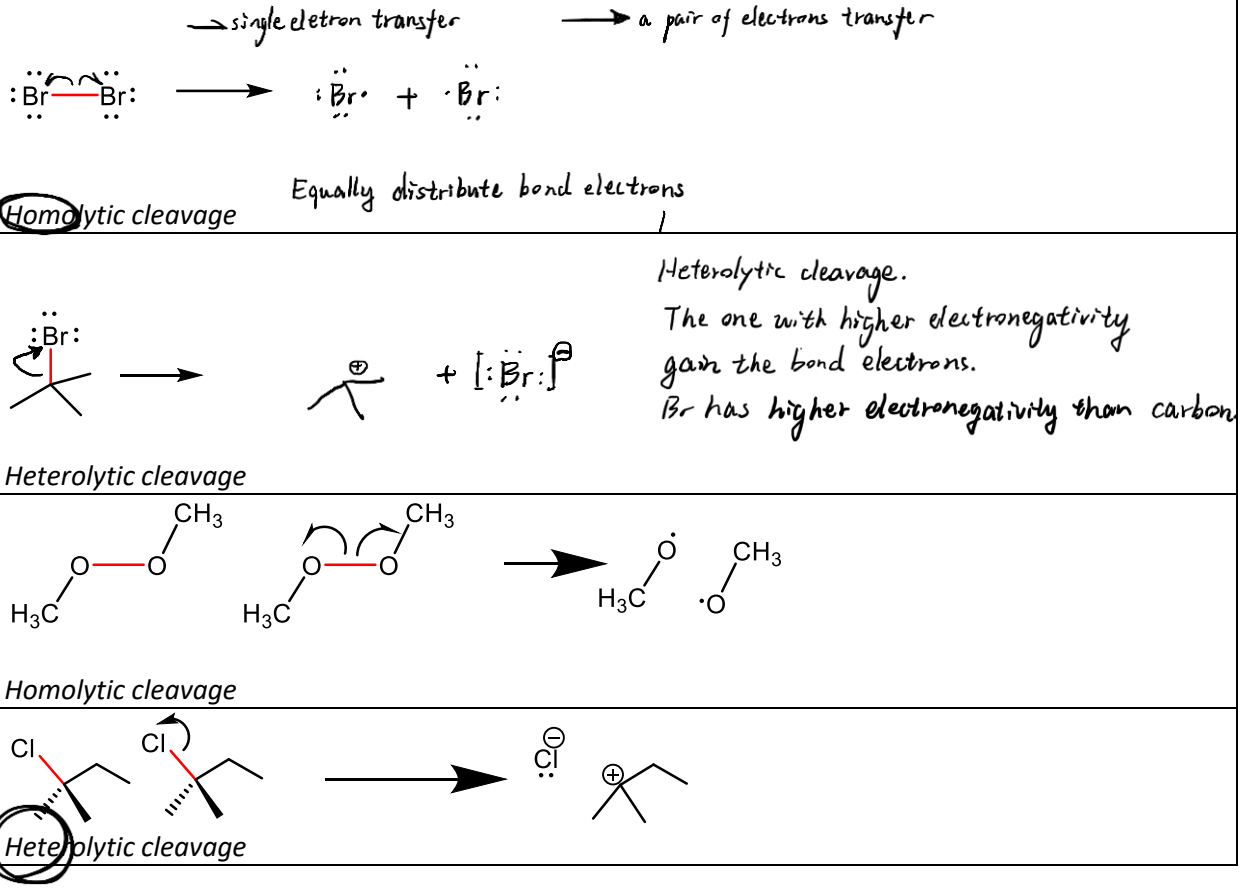
Question 1. Label each reaction event below with either the bonding-breaking type or the specific reaction type. Choose the type that **best** describes the reaction event drawn.
Choices: substitution, addition, elimination, heterolytic cleavage, homolytic cleavage

Reaction scheme	Reaction type (one **best** choice)
	Substitution
	Homolytic cleavage
	Addition
	Elimination

Question 2. Break the red bond of the following molecules in either a homolytic or heterolytic fashion, as indicated. Show the cleaved products produced with the appropriate electrons and charge. Be sure to draw in the correct arrows to show the movement of electrons.
a)



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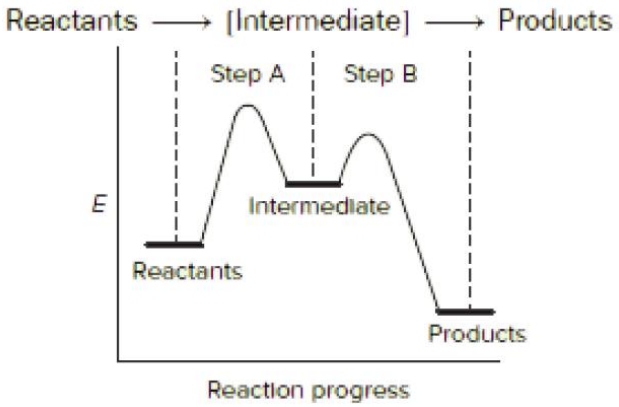
Question 3. Answer the questions below based on the following reaction energy diagram

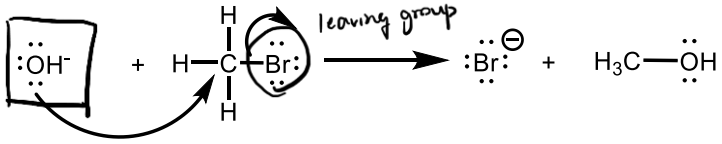
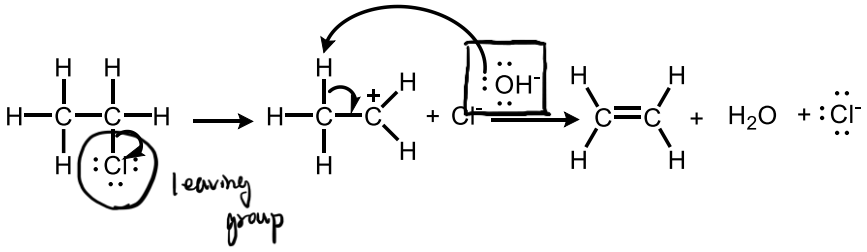


i. Is the reaction concerted or stepwise?
Stepwise – intermediate is formed

ii. Is the reaction endothermic or exothermic overall?
Exothermic – products are lower in the energy than reactants, so energy is released.

iii. How many transition states are there in this reaction pathway?
2 transition states – Peaks of A and B

Question 4. Identify the mechanism below as either S_N1, S_N2, E2 or E1. Circle the leaving group in each reaction. Put a square around the nucleophile.

Reaction mechanism	**Mechanism type**
 Leaving group is the one that leaves. It is always nucleophile that attacks electrophile. The arrows points away from the nucleophile to the electrophile.	SN2
 Leaving group: Cl-; Nucleophile: OH-; Electrophile: Carbon centre	E1 because a carbocation intermediate is being attacked by the nucleophile

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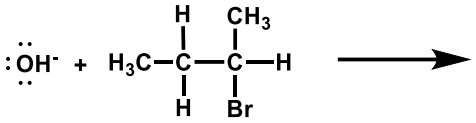
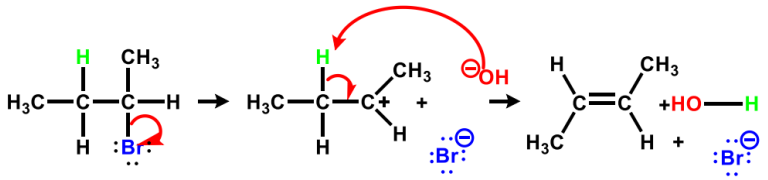
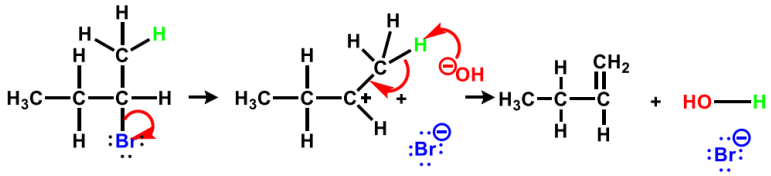
Question 5. Draw the mechanism of reaction and the product formed resulting from an <u>E1</u> reaction of the following reactant and substrate:



Note we haven't gone over which position to put the double bond, so either of these would be accepted! Make sure the intermediate is indicated!

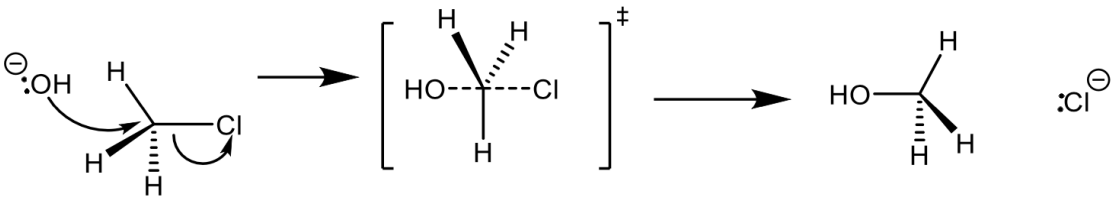


intermediate

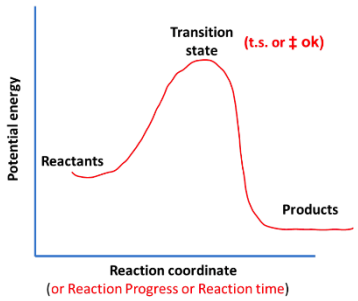


intermediate

Question 6. a) Provide the detailed mechanism of the SN2 reaction of methylchloride with a sodium hydroxide. Include any transition states or intermediates of the reaction. Use arrows to indicate the flow of electrons and indicate any charge/lone pairs that are important.



b) Assume that the SN2 reaction above is exothermic, draw the associated reaction energy diagram for this reaction. Include all the necessary labels.



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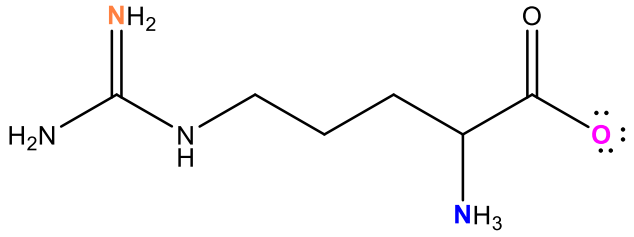
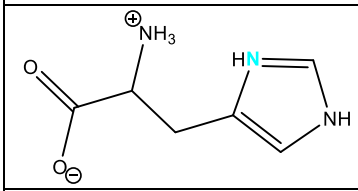
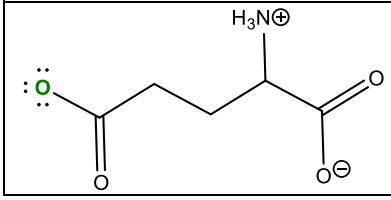
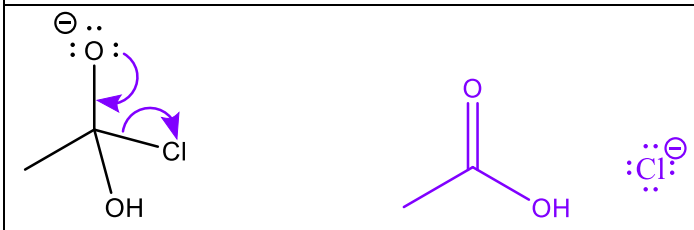
Question 7. What is the formal charge on each indicated atom? Show the calculation.

	N Neutral valence is 5 Assigned electrons = 4 (4 bonds) 5-4=1, FC = +1 N Neutral valence is 5 Assigned electrons = 4 5-4=1, FC = +1 O Neutral valence is 6 Assigned electrons = 7 6-7=-1, FC = -1
	N Neutral valence is 5 Assigned electrons = 4 5-4=1, FC = +1
	O Neutral valence is 6 Assigned electrons = 7 6-7=-1, FC = -1

Question 8. Draw the product(s) of the arrow pushing.



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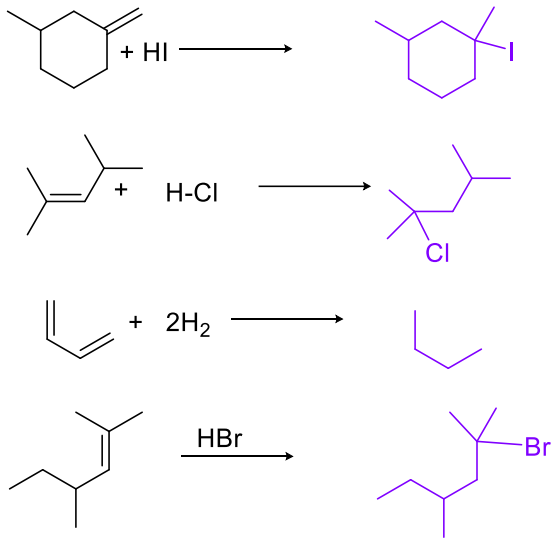
Question 9. Draw the products of the reactions.



Question 10. Which is the better nucleophile from each pair and why?

NH_2^- vs NH_3	NH_2^-: They are basically the same species (and atom donating the electrons is N in both cases) so the one that is negatively charged is better able to donate electrons
Br^- vs Cl^-	Br^-: Same group on the periodic table, so when you go down a group the electrons are in a higher energy shell and are thus more polarizable
OH^- vs NH_2^-	NH_2^- : Both are negative, and you are going across the periodic table… as such the central atom N is the least electronegative and therefore more likely to donate its electrons to the reaction