**CHE2060 Lecture 7 HW: Reaction mechanism overview**

Problems must be solved, or written out, in their entirety with all work shown on engineering graph paper. You must label each set in the upper left hand corner with your name, the date and the chapter. Problems must be identified by number and all work must be shown with answers boxed.

**7.1: Reaction energies & transition states**

1. Rank the relative energies of:

a. reactants

b. transition states

c. products

Lowest to highest: products < reactants < transition states

2. What is activation energy?

Activation energy is the energy required to transform reactants into transition states. Input of energy is required because the energy state of the reactants is lower than the energy state of the transition state. The transition state is a high energy, unstable molecule or ion.

**7.2: Review of acid-base reaction mechanisms**

3. In an acid-base reaction, which attacks, the electrophile or the nucleophile?

In acid base reactions, the electron pair of the nucleophile ‘attacks’ the electrophile to quench the positive (or dipolar positive) charge and form a dative bond.

4. What two numbers can you use to determine whether the reactants or products of a reaction are favored?

1. Compare the pKa of the acid and conjugate acid. The acid with the lower pKa pushes

 the reaction away from it and towards the acid with the higher pka.

2. Keq values of over one favor products while Keq values of less than one favor

 reactants.

5. What is a ‘leaving group’?

A leaving group is an atom (or group of atoms) that leaves a molecule, taking its electron pair with it.

**7.4: Substitution reactions**

6. In each reaction, is the nucleophile the substrate or reactant?

a. SN1 reactions reactant

b. SN2 reactions reactant

c. electrophilic substitutions substrate

7. Substitution: 2-chloropentane + water 🡪

1. Draw line-bond structures of the substrate and reactant;
2. Identify Nu: and E+ when appropriate;
3. What type of substitution mechanism occurs?
4. Predict the product and by-product on the right & draw their line-bond structures;
5. Use arrows to show the movement of electrons needed to create the products and use as many steps as needed – be sure to show any intermediates;
6. Re-write each reaction in a simplified form, showing reactant above the arrow and by-product leaving at the arrow; and
7. Does the reaction create any new chiral carbon(s)?

SN1



8. Substitution: 2-chloropentane + hydroxide ion

1. Draw line-bond structures of the substrate and reactant;
2. Identify Nu: and E+ when appropriate;
3. What type of reaction mechanism occurs
4. Predict the product and by-product on the right & draw their line-bond structures;
5. Use arrows to show the movement of electrons needed to create the products and use as many steps as needed – be sure to show any intermediates;
6. Re-write each reaction in a simplified form, showing reactant above the arrow and by-product leaving at the arrow; and
7. Does the reaction create any new chiral carbon(s)?

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**7.5: Addition reactions**

9. In addition reactions, atoms or groups are added to substrates from reactants. Yet, no atom or group leaves the substrate. How or why is that possible?
No groups leave because addition removes a double bond; an unsaturated substrate becomes saturated as new components are added “across” a double bond.

10. Addition: 2-hexene + HCl

1. Draw line-bond structures of the substrate and reactant;
2. Identify Nu: and E+ when appropriate;
3. What type of addition reaction is this?
4. Predict the product and by-product on the right & draw their line-bond structures;
5. Use arrows to show the movement of electrons needed to create the products and use as many steps as needed – be sure to show any intermediates;
6. Re-write each reaction in a simplified form, showing reactant above the arrow and by-product leaving at the arrow; and
7. Does the reaction create any new chiral carbon(s)?



11. Addition:

1. Identify Nu: and E+ when appropriate;
2. What type of addition reaction is this?
3. Predict the product and by-product on the right & draw their line-bond structures;
4. Use arrows to show the movement of electrons needed to create the products and use as many steps as needed – be sure to show any intermediates;
5. Re-write each reaction in a simplified form, showing reactant above the arrow and by-product leaving at the arrow; and
6. Does the reaction create any new chiral carbon(s)?





**7.6: Elimination reactions**

12. Elimination reactions remove atoms or groups that become by products and create products with what common characteristic?

Double bonds or triple bonds; additional unsaturation

13. Elimination:



1. Identify Nu: and E+ when appropriate;
2. Predict the product and by-product on the right & draw their line-bond structures;
3. Use arrows to show the movement of electrons needed to create the products and use as many steps as needed – be sure to show any intermediates;
4. Re-write each reaction in a simplified form, showing reactant above the arrow and by-product leaving at the arrow; and
5. Does the reaction create any new chiral carbon(s)?

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14. Elimination:

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1. Identify Nu: and E+ when appropriate;
2. Predict the product and by-product on the right & draw their line-bond structures;
3. Use arrows to show the movement of electrons needed to create the products and use as many steps as needed – be sure to show any intermediates;
4. Re-write each reaction in a simplified form, showing reactant above the arrow and by-product leaving at the arrow; and
5. Does the reaction create any new chiral carbon(s)?

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**~~7.7: Competition between substitution, addition & elimination reactions~~**

~~15. When a number of different reaction mechanisms are possible, what does the nature of the substrate determine?~~

~~The substrate determines whether an addition or elimination reaction occurs. Alkanes can undergo eliminations but not additions. Alkenes can undergo additions.~~

~~16. When a number of different reaction mechanism are possible, what does the nature of the nucleophile determine?~~

~~The nature of the nucleophile determines whether substitution or elimination reactions occur. Sulfuric or phosphoric acids favor elimination while hydrochloric acid favors substitutions.~~