EXAM 3 study guide

Organic Chemistry 2e chapters 7-8, 15

**DAY 15, Terms to know**:

Sections 7.1-7.5 Substitution reaction, leaving group, alkyl halide, primary, secondary, tertiary, SN2, inversion of stereochemistry, concerted, step-wise, backside attack, SN1, retention of stereochemistry, racemization of stereochemistry, slow step or rate determining step

**DAY 15, Specific outcomes and skills that may be tested on exam 3:**

Sections 7.1-7.5

* Be able to predict which side of a substitution reaction will be favored based on the stability of products versus reactants and changes in entropy for reactants and products
* Be able to correctly draw and label a reaction coordinate diagram for a substitution reaction.
* Be able to draw mechanism arrows on a given substitution reaction and label the nucleophile and leaving group.
* Be able to describe the key characteristics that make a leaving group GOOD and rank leaving groups in terms of their ability to leave.
* Be able to name an alkyl halide using the IUPAC sysem, and be able to draw an alkyl halide from its name.
* Be able to identify some specific alkyl halides based on their common names (see slide 7-8)
* Be able to identify primary, secondary, and tertiary alkyl halides and be able to identify the alpha, beta, gamma, and delta carbons on the alkyl chain of an alkyl halide.
* Be able to draw mechanism arrows for an SN2 reaction and be able to identify a reaction with arrows as either SN2 or SN1.
* Be able to write a correct rate law for an SN2 reaction.
* Be able to identify an SN2 reaction based on inversion of stereochemistry.
* Given reactants and knowing they undergo SN2, be able to predict products with the proper stereochemical configuration.
* Be able to draw a reasonable transition state for an SN2 reaction.
* Be able to recognize and explain why steric hindrance affects the reaction rate for SN2 reactions.
* Be able to recognize and explain why the strength of the nucleophile affects the rate of SN1 reactions.
* Be able to draw and label a correct reaction coordinate diagram for any substitution reaction.
* Given a reaction coordinate diagram, be able to make both kinetic and thermodynamic arguments about SN2 reactions.
* Be able to draw mechanism arrows for an SN1 reaction..
* Be able to write a correct rate law for an SN1 reaction.
* Be able to identify that the first step of an SN1 reaction is always the slow step and b e able to explain how that affects the rate law of a reation.
* Be able to explain how you could run a kinetics experiment in the lab to determine if a substitution reaction were running by SN1 or SN2.
* Be able to explain how you could run a stereochemical experiment in the lab to determine if a substitution reaction were running by SN1 or SN2.
* Be able to identify an SN1 reaction based on racemization of stereochemistry.
* Given reactants and knowing they undergo SN1, be able to predict products with the proper stereochemical configuration.
* Be able to draw reasonable transition states for each step of an SN1 reaction.
* Be able to recognize and explain why steric hindrance affects the reaction rate for SN1 reactions.
* Be able to recognize and explain why carbocation stability affects the rate of SN1 reactions.
* Be able to recognize and explain why the quality of the leaving group affects the rate of SN1 reactions.
* Given a reaction coordinate diagram, be able to make both kinetic and thermodynamic arguments about SN1 reactions.

**DAY 16, Terms to know**:

Sections 7.6-7.9 solvolysis, benzyl, aryl, sulfonate ions, protic solvent, aprotic solvent

**DAY 16, Specific outcomes and skills that may be tested on exam 3:**

Sections 7.6-7.9

* Be able to identify when proton transfer steps are necessary prior to loss of a leaving group in substitution reactions and be able to use proper arrows to show electron movement for such steps.
* Be able to identify when proton transfer steps are necessary after the loss of a leaving group and nucleophilic attack in substitution reactions and be able to use proper arrows to show electron movement for such steps.
* Be able to draw a complete mechanism for substitution reactions and be able to use thermodynamic principles to predict whether each step in the mechanism (as well as the entire reaction) is product favored or reactant favored.
* Be able to explain conditions under which it is appropriate to use the nulceophile also as the solvent for a reaction and why such solvolysis may allow the reaction to be more product favored than it would be otherwise.
* Be able to identify situations where rearrangement steps occur in substitution reactions and correctly draw mechanisms and predict products for such reactions.
* Given reactants and products, predict a set of reagents and solvents that would be most appropriate for the desired reaction.
* Be able to recognize allyl, vinyl, benzyl, and aryl sites and how such sites affect the stability of a carbocation in a proposed SN1 reaction.
* Be able to assess the strength of the nucleophile and how the solvent used affects the nucleophile’s strength in a substitution reaction and what impact that will have on whether the reaction goes by an SN1 or an SN2 mechanism.
* Be able to explain what makes sulfonates such great leaving groups.
* Be able to thoroughly describe the role of the solvent in a substitution reaction and how it interacts with the reactants, transitions states, intermediates, and products.
* Be able to explain how the polarity or the solvent and whether it is protic affects the mechanism of the substitution reaction.
* Be able to give examples of solvents that fit each of the following categories: polar protic, polar aprotic, nonpolar.
* For a specific desired product, be able to give the best reaction conditions including nucleophile, substrate with leaving group, solvent, and temperature.

**DAY 17, Terms to know**:

Sections 8.1-8.7regio Elimination reaction, alkene, Bredt’s rule, E/Z notation, E1, E2, Zaitsev product, Hofmann product, regioselectivity

**DAY 17, Specific outcomes and skills that may be tested on exam 3:**

Sections 8.1-8.7regio

* Be able to compare and contrast bases and nucleophiles.
* Be able to predict products given reactants and reagents for an elimination reaction including regioselectivity concerns.
* Be able to name a given alkene or draw an alkene given its name.
* Be able to differentiate between cis and trans isomers in alkenes.
* Be able to apply and explain Bredt’s rule for syclic and bicyclic alkenes.
* Be able to use proper E/Z notation with alkenes, and be able to determine where cis and trans notation is not appropriate and E/Z is.
* Be able to assess the stability of alkenes based on degree of substitution, sterics, and number of pi vs sigma bonds.
* Be able to relate stability and heat of combuistion.
* Be able to draw both E1 and E2 mechanisms with proper arrow pushing.
* Be able to explain how the identity of the base/nucleophile used either promotes E1 or E2.
* Be able to explain how the identity of the electrophile (sterics and quality of leaving group) used either promotes E1 or E2.
* Be able to explain how the identity of the base/nucleophile used either promotes elimination or substitution.
* Be able to explain how the identity of the electrophile (sterics and quality of leaving group) used either promotes elimination or subsitution.
* Given the mechanism, be able to give the correct rate law for an elimination and explain why.
* Given information about the rate law for a reaction, be able to distinguish between E1 and E2 and explain why.
* Be able to draw transition states for each step in an E1 or E2 reaction and explain how the properties of the reactant and substrate affect the stability of the transition state and thus the rate of one mechanism vs. another.
* Be able to choose an appropriate base that will give desired regioselectivity for an elimination reaction.
* Be able to make a kinetic vs. thermodynamic argument to explain regioselectivity in elimination reactions.

**DAY 18, Terms to know**:

Sections 8.7stereo-8.12 stereoselective, stereospecific, coplanar, anti-coplanar, syn-coplanar, anti-periplanar, polarizability

**DAY 18, Specific outcomes and skills that may be tested on exam 3:**

Sections 8.7stereo-8.12

* Given reactants for an elimination reaction, be able to correctly predict major and minor products based on stereoselectivity and explain WHY.
* Be able to correctly predict E2 products that can and cannot form based on stereospecificty and explain WHY.
* Be able to determine possible products and major products for E2 reactions when the leaving group is attached to a cyclohexane ring recognizing that the transition state must go through an anti-periplanar geometry and WHY.
* Be able to identify the rate determining step in E1 reactions and explain why and how that affects the rate law.
* Be able to explain ways to promote E1 over SN1 and vice versa based on kinetics and thermodynamics.
* Be able to recognize and explain why E1 reactions nearly always give the Zaitsev product and cannot be manipulated to give the Hofmann product predominantly.
* Be able to correctly predict whether E1 reactions will give E or Z products and explain why.
* Be able to recognize where and why proton transfer steps and rearrangement steps are necessary in elimination reactions.
* Be able to recognize how charge, polarizability, and sterics affect how a reactant reacts strong vs. weak, nucleophilic, vs. basic and why. Also, be able to use that information to distinguish when a reaction is likely to be elimination vs. substitution.
* Be able to predict products in a reaction given reactants that are likely to undergo either SN1, SN2, E1, or E2.
* Be able to use p*K*a values for conjugate acids to quantify the strengths of bases.
* Be able to use ARIO to assess qualitatively the strengths of bases.

**DAY 19, Terms to know**:

Sections 8.13-8.14, 15.1-15.4 Spectroscopy, photons, wavelength, frequency, quantum behavior, spectrophotometer, % transmittance, wavenumber

**DAY 19, Specific outcomes and skills that may be tested on exam 3:**

Sections 8.13-8.14, 15.1-15.4

* Be able to explain the relationships between wavelength, frequency, and energy for light.
* Be able to rank the different categories of light radiowaves, microwaves, IR, UV, etc.) based on energy, wavelength, or frequency.
* Be able to explain the differences between continuous behavior and quantum behavior.
* Be able to explain how vibration, rotation, and energy of electrons are all quantized.
* Be able to explain what happens in general when IR light hits a molecule.
* Be able to explain what happens to the energy when a molecule excited by IR light relaxes.
* Be able to explain why objects emit IR radiation how that relates to temperature.
* Be able to give a description of how a spectrophotometer works and how it gives information about the structure of a compound.
* Be able to explain how wavenumber and intensity relate to the type of bond absorbing the radiation.
* Be able to explain how bond strength and length relate to the wavenumber observed in stretching IR frequencies.
* Be able to analyze an IR spectra and pick out the most relevant peaks and determine what information about the molecule can be determined from the analysis of those peaks.
* Be able to explain the significance of the region around 3000 cm-1 and how that relates to the type of atom and hybridization of the atom bonded to a hydrogen atom.
* Be able to explain how the intensity of a signal relates to the polarity of the bond and the number of bonds present giving the signal.

**DAY 20, Terms to know**:

Sections 15.5-15.16 diagnostic region, fingerprint region, primary amine, secondary amine, tertiary amine, mass spectrometry (MS), ionization, electron impact (EI), radical cation, molecular ion, fragmentation, base peak, electrospray, soft vs. hard ionization, degrees of unsaturation or hydrogen deficiency index (HDI)

**DAY 20, Specific outcomes and skills that may be tested on exam 3:**

Sections 15.5-15.16

* Be able to explain how shape in IR spectra relates to the type of bond absorbing the radiation.
* Be able to explain how H-bonding affects signals involving stretching of H atoms bonded to heteroatoms.
* Be able to explain how N-H stretching works for both primary and secondary amines.
* Given a molecule, be able to predict the key IR stretching peaks that would be observed.
* Be able to explain how two molecules can be distinguished by differences in their IR spectra.
* Be able to explain how ionization and detection of mass occurs in MS.
* Be able to explain how the molecular ion forms in MS and how and why fragmentation often occurs.
* Be able to explain why only charged molecules and fragments are observed in MS.
* Be able to explain why the (M+1)+ peak is seen in MS and how its height relative to the M+ peak relates to the number of carbons in the molecule.
* Be able to recognize the presence of Cl or Br in a compound based on MS data and the isotopic distribution.
* Be able to use given data about the MS and IR to conclude information about a compound’s formula, degrees of unsaturation, and ultimately its structure.