# List of Objectives for Organic Chemistry I

Changes made during the semester will be made in red.

Things you should be able to do from Ch. 1 sections 1-12:

|  |  |
| --- | --- |
| 1 | Draw the shape of s and p orbitals. |
| 2 | Determine ground state electronic configurations of atoms. |
| 3 | Determine how many valance electrons are present in atoms and molecules. |
| 4 | Draw complete Lewis dot structures that include all lone pair electrons and formal charges if any are present. |
| 5 | Label bonds as ionic or covalent. |
| 6 | Use wedges (“solid wedge”) and dashes (“dashed wedge”) to represent molecules in 3-D. We will emphasize this more in coming chapters. |
| 7 | Label hybridization (i.e. sp3), geometry (i.e. tetrahedral), and approximate bond angles (i.e. 109.5°) for organic molecules. |
| 8 | Describe/diagram sigma and pi bonds. |
| 9 | Understand some basic differences between Molecular Orbital Theory and Valence Bond Theory MO theory discusses orbitals in molecules in terms of bonding and anti-bonding. Valence bond theory discusses orbitals in molecules as hybridized atomic orbitals (i.e. sp, sp2, sp3). Valence bond theory is often used to explain geometries and reactivities of organic molecules, and it is the model we will use most frequently. MO theory is a more mathematically correct model and is used by physical chemists and some specialties of organic chemistry, such as the computational chemistry used in the Spartan molecular modeling programs. |
| 10 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 2 sections 1-6:

|  |  |
| --- | --- |
| 1 | Rank atoms by electronegativity. |
| 2 | Recognize and label bond polarity and dipoles. |
| 3 | Determine the direction of bond dipoles and molecule dipole moments. |
| 4 | Determine if a molecule will have a dipole moment. |
| 5 | Calculate formal charges. |
| 6 | Draw reasonable major and minor resonance contributors. |
| 7 | Rank resonance contributors by importance. |
| 8 | Use electron-pushing arrows. Show how electrons move from resonance structure A to resonance structure B or, if given electron-pushing arrows, show the indicated resonance contributor. Electron-pushing arrows ALWAYS start at electrons! (More with acid/base chemistry and in Ch. 5 section 6.) |
| 9 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 3:

|  |  |
| --- | --- |
| 1 | Recognize organic functional groups or draw a molecule representative of a given functional group. |
| 2 | Use IUPAC nomenclature to name straight chain and branched alkanes and cycloalkanes. |
| 3 | Name or draw molecules using the common names isopropyl, isobutyl, sec-butyl, or tert-butyl. |
| 4 | Provide a structure for branched alkyl group, such as 3-methylbutyl, if given the name. |
| 5 | Label carbons as primary, secondary, tertiary (or quaternary – a carbon bonded to 4 other carbons) |
| 6 | Understand that hydrocarbons combust in the presence of O2 to give CO2, H2O, and heat. The amount of heat given off is directly proportional to the amount of energy stored in the bonds of the molecule. |
| 7 | Rank molecules by boiling point or solubility in a given solvent based on the 3 types of intermolecular interactions. A) London dispersion forces (the weakest) between molecules that do not contain permanent dipoles B) dipole-dipole interactions and C) hydrogen bonding (the strongest). We will explore intermolecular interactions to a greater extent in later chapters.  *Note: I often refer to (A) as van der Waals forces. Technically, (A) and (B) are both classified as van der Waals interactions.* |
| 8 | Rank isomeric alkanes by stability. Generally for alkanes, the more highly branched alkane is more stable. Thus, it has lower potential energy, less energy stored in the bonds, and lower heat of combustion. |
| 9 | Rank alkanes, including isomers, by boiling point. |
| 10 | Draw constitutional isomers of simple organic molecules of a given molecular formula without duplicating structures. |
| 11 | Recognize that cycloalkanes have cis/trans isomers but alkanes do not. (Models may be helpful.) |
| 12 | Use/Draw Lewis structures, condensed structural formulas, and line structures (skeletal structures) to represent a molecule. (See Ch. 2 section 12.) |
| 13 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 4:

|  |  |
| --- | --- |
| 1 | Draw, recognize, and interconvert staggered and eclipsed conformations drawn as wedge-and-dash structures, sawhorse formulas, or Newman projections. |
| 2 | Rank relative energies of conformational isomers. |
| 3 | Indicate dihedral angles of staggered and eclipsed conformations shown in any 3-D representation. |
| 4 | Draw a clearly labeled potential energy diagram for a conformational analysis (as on p.106.) |
| 5 | Recognize sources of strain in small rings. |
| 6 | Draw substituted cyclohexanes in both chair conformations clearly showing all axial and equitorial groups, including H’s. (You should be able to flip the chair.) |
| 7 | Rank relative energies of one compound in each of its chair conformations or two compounds in a given chair conformation. |
| 8 | Draw the lowest energy conformation of a multi substituted cyclohexane. |
| 9 | Draw cis and trans disubstituted rings. |
| 10 | Recognize/identify cis-decalin vs. trans-decalin structures. (You will not be asked to draw the decalin bicyclic ring system.) |
| 11 | Provide IUPAC names for simple bicycloalkanes (such as bicyclo[2.2.1]heptane.) |
| 12 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 9:

|  |  |
| --- | --- |
| 1 | Visualize and draw molecules in 3-D. That includes being able to rotate around bonds and draw the resulting structure. You should be able to interconvert molecules drawn as wedge-and-dash, Newman projections, sawhorse formulas, and Fischer projections. |
| 2 | Recognize whether a molecule is chiral or achiral. |
| 3 | Name compounds that contain chiral centers, including R or S configuration. |
| 4 | Recognize symmetry within molecules. If a molecule has a plane of symmetry (a mirror plane within the molecule), it will be superposable on its mirror image, achiral, and optically inactive. |
| 5 | Determine whether or not a compound will be optically active (and thus rotate plane-polarized light.) All chiral compounds will rotate plane-polarized light. |
| 6 | Use the equation =[]D x C x l |
| 7 | Calculate %ee (enantiomeric excess) if given the observed rotation of a mixture of enantiomers and the specific rotation of one of those enantiomers. |
| 8 | Calculate the enantiomeric composition of a mixture if given the %ee. |
| 9 | Recognize stereocenters (or chirality centers or stereogenic centers) and assign absolute configurations (R or S) to each using the Cahn-Ingold-Prelog priorities. (See section 9.5 and 6.6.) |
| 10 | Calculate the number of stereoisomers that are possible for a given compound. (Recognize presence of meso compounds.) |
| 11 | After ch. 6 material is covered, recognize stereoisomers (diastereomers) in alkenes. Be able to name alkenes as cis/trans or Z/E. A compound with one chiral center and an alkene can have 4 stereoisomers: 1) R and Z, 2) R and E, 3) S and Z, 4) S and E. All 4 are related to each other as diastereomers. |
|  | \*Identify the relationship between pairs of compounds as enantiomers, diastereomers, constitutional isomers, two molecules of the same compound or not isomers at all. (See 9.11.) The molecules may be drawn in any 3-D way, including wedge-and-dash, Newman projections, sawhorse formulas, and Fischer projections. |
|  | Draw an enantiomer, diastereomer, constitutional isomer, and/or conformational isomer of a given compound. |
|  | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 13:

|  |  |
| --- | --- |
| 1 | Predict whether or not a nucleus will be NMR active. |
| 2 | Recognize that nuclear spin flips in the presence of an external magnetic field require energy input that corresponds to the energy of radio frequency. |
| 3 | Understand shielding. Electron density around an atom can shield that atom from the external magnetic field. As a result, atoms bound to electronegative atoms are deshielded and the signals for such atoms appear downfield (to the left) in the NMR spectrum. |
| 4 | Recognize that magnetic anisotropy results from the movement of electrons in -bonds. The resulting magnetic fields typically cause deshielding on atoms near -bonds. |
| 5 | Predict the number of separate signals that would be observed in the 13C NMR or 1H NMR of a given compound by recognizing equivalent groups or atoms in the molecule. |
| 6 | Label atoms in a molecule that are 3-bond neighbors. (H’s that are related as 3-bond neighbors typically split one another.) |
| 7 | Predict the splitting patterns for each type of proton present in the 1H NMR. |
| 8 | Use Pascal's triangle (which would not be provided) to predict the relative intensities of peaks within a defined coupling pattern. (i.e., a triplet is 1:2:1, a quartet is 1:3:3:1, etc.) |
| 9 | Be able to use 13C NMR data to assist you in solving the structure of an unknown. |
| 10 | \*Be able to interpret and predict 1H NMR spectra. You should have a general understanding of chemical shift, integration, and spin-spin coupling in 1H NMR. |
| 11 | Sketch the expected 1H NMR of a given compound including approximate chemical shift, splitting patterns, integrations, and assignments. |
| 12 | Recognize that OH’s can be exchanged to OD’s, allowing you to verify the presence (then absence) of an OH in the 1H NMR spectrum. |
| 13 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 12:

|  |  |
| --- | --- |
| 1 | Rank portions of the electromagnetic spectrum in terms of energy. (For example, infrared radiation is less energetic than ultraviolet radiation.) |
| 2 | Memorize the equations  = *c*/ and = *h*. |
| 3 | Know that infrared radiation excites stretching and bending of bonds. |
| 4 | Recognize that higher wavenumber corresponds to higher energy. |
| 5 | \*Interpret infrared spectra by clearly identifying absorbances. Be able to recognize which functional group or groups are present in a molecule. (IR excites stretching and bending of bonds, not hybridized atoms. Keep that in mind when assigning absorbances.) |
| 6 | \*Match IR spectra to particular compounds from a list of compounds that contain different functional groups. |
| 7 | Label prominent peaks in a given IR spectrum (from the in class handout of major and minor peaks.) |
| 8 | Indicate specifically how you could differentiate molecules from each other using either IR or NMR spectroscopy. |
| 9 | \*\*Be able to combine IR, NMR, and molecular formula to solve the structure of an unknown. (If given the molecular formula, it is always a good idea to FIRST solve for the degree of unsaturation.) |
| 10 | All recommended and/or required problems and problems similar to them. |

We will not cover mass spectrometry in lecture. You may find sections 12.1-12.4 helpful for lab.

**Cutoff for Exam 1 material.**

Things you should be able to do from Ch. 2 sections 7-11 and from the acid/base handout that is posted on my web page:

|  |  |
| --- | --- |
| 1 | Define/recognize Bronsted-Lowry acids and bases. |
| 2 | Define Ka and pKa. (Show equations that would be used to calculate each.) |
| 3 | Use pKa values to determine the predominant direction of a reaction at equilibrium. |
| 4 | Arrange chemical species in order of increasing acidity or basicity. Weigh importance of factors that influence acidity (bond energies, electronegativity, inductive effects, RESONANCE, and hybridization). |
| 5 | Add electron-pushing arrows to a given acid/base reaction or give the products of any reaction if given the electron-pushing arrows. (A few copies of an electron-pushing workbook are on reserve in the library for your use.) |
| 6 | \*Draw products of Bronsted-Lowry acid/base reactions, label acid and base on each side of reaction, and determine predominant direction of equilibrium **without** pKa tables. You should know approximate pKa’s of organic functional groups (carboxylic acids, alcohols, amines, and alkanes.) |
| 7 | Define/recognize Lewis acids and bases. |
| 8 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 5:

|  |  |
| --- | --- |
| 1 | Identify reactions by type: addition, elimination, substitution, or rearrangement. |
| 2 | Draw electron-pushing arrows for homolytic and heterolytic steps of a reaction. If given reagents and products, you should be able to provide missing arrows. |
| 3 | Use electronegativity of atoms to determine bond dipoles and which atoms in a molecule will be electron rich and which will be electron poor. |
| 4 | Identify electrophiles and nucleophiles either by themselves or in a given complete reaction. |
| 5 | Understand some basics about Keq, G, H, and S. In particular, reactions are favorable when Keq is greater than one, when G is negative, when H is negative, and when S is positive. (See Table 5.2.) |
| 6 | Understand/explain the difference between kinetics (reaction rates) and thermodynamics (reaction equilibria). Kinetics will tell you how fast a reaction will occur. Thermodynamics will tell you if the reaction is favorable energetically. |
| 7 | Calculate bond dissociation energies of reactions and use the calculation to predict whether the reaction would be endothermic (unfavorable) or exothermic (favorable.) If asked to do such a calculation, you would be provided with a table such as Table 5.3. |
| 8 | Draw a reaction energy diagram if told that the reaction is endothermic or exothermic, how many steps are involved in the reaction, and which step is rate-determining. |
| 9 | Label activation energy and location of starting materials, transition state, (and intermediates if multiple transition states), and products on a reaction energy diagram. |
| 10 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 6:

|  |  |
| --- | --- |
| 1 | Calculate the degree (or units) of unsaturation for molecules containing C, H, O, N, and halogens. |
| 2 | Name alkenes. |
| 3 | Draw alkenes if given the name. |
| 4 | Rank substituents on each carbon involved in a C-C -bond by the Cahn-Ingold-Prelog rules and then determine if an alkene has an E or Z configuration. |
| 5 | Identify methylene, vinyl, and allyl groups. |
| 6 | Draw a 3-D representation of overlapping p-orbitals showing the -bonding in an alkene. |
| 7 | Either rank alkenes in order of stability or match a list of alkenes with the appropriate heats of hydrogenation or combustion. (It’s the same concept.) |
| 8 | Predict the products of catalytic hydrogenation experiments (alkene + H2/catalyst → alkane). |
| 9 | Clearly show (in 3-D) that the addition of H2 is a syn-addition. |
| 10 | Label alkenes as either mono-, di-, tri-, or tetra-substituted. |
| 11 | Rank carbocations in order of stability. NEVER propose methyl or primary carbocations as intermediates in reactions! |
| 12 | Predict the products of electrophilic addition reactions of HX to an alkene. You should also be able to do the reaction in reverse. If given an alkyl halide, you should be able to determine what HX and alkene could be used to synthesize the alkyl halide. |
| 13 | Predict products of electrophilic addition reactions of HX to unsymmetrical alkenes using Markovinikov’s rule. |
| 14 | Provide a mechanism for a reaction that involves a carbocation rearrangement. (Recognize when carbocation rearrangements will be thermodynamically favorable.) |
| 15 | \*Provide a reaction energy diagram (Potential Energy vs. Reaction Coordinate) for any of the reactions covered in ch. 6. |
| 16 | All recommended and/or required problems and problems similar to them. |

Hammond’s Postulate will be covered in the Spartan Pinacolone lab.

Things you should be able to do from Ch. 7:

|  |  |
| --- | --- |
| 1 | Predict the products of the dehydration of an alcohol in the presence of acid or the dehydrohalogenation of an alkyl halide in the presence of base. (See 7.1.) |
| 2 | Draw the structure of tetrahydrofuran, THF. (See page 215.) |
| 3 | \*Draw products of reactions of alkenes with the reagents discussed in Ch. 7 (Cl2, Br2, NBS as a source of Br2, X2/H2O, X2/ROH, H2O/H+, Hg(OAc)2/H2O/THF followed by NaBH4, BH3, BH3 followed by H2O2/HO-, H2/catalyst, OsO4, OsO4 (1 equivalent) followed by NaHSO3 or OsO4 (catalytic) with H2O2/H2O or N-methylmorpholine N-oxide (NMO), O3, O3 followed by oxidative or reductive workup, KMnO4, and RCO3H. Draw the products and mechanisms of reactions of alkenes with HBr/peroxides ~~or N-bromosuccinimide (NBS)~~. |
| 4 | Draw the products and mechanisms of alkene radical polymerizations. Or, if given a polymer, determine the alkene that was used to make it. (See 7.10.) |
| 5 | Clearly show stereochemistry of products when necessary.   * hydrogenation: syn addition of H2 * hydroboration-oxidation: syn addition of H and OH * halogenation: anti addition of X2 (or X and OR). Regiochemistry is also important if X2/ROH is added to an unsymmetrical alkene. The OR bonds to the more highly substituted carbon. |
| 6 | Clearly show the regiochemistry of addition reactions.   * In the absence of peroxides, concentrated acids (HX) will add to alkenes with a Markovnikov regioselectivity to give alkyl halides. * In the presence of peroxides, concentrated acids (HX) will add to alkenes with an anti-Markovnikov regioselectivity to give alkyl halides. * Water can add across a C=C with a Markovnikov regioselectivity yielding alcohols. (Hg(OAc)2/H2O/THF followed by NaBH4) * Water can add across a C=C with anti-Markovnikov regioselectivity yielding alcohols. (BH3 then H2O2/NaOH/H2O) |
| 7 | Draw the product of the reaction of a vicinal diol with HIO4. |
| 8 | Provide the missing starting material(s) if given one reagent and the product or just the product. |
| 9 | \*Provide mechanisms for most of the reactions covered in Ch. 7. You do NOT need to know electron-pushing mechanisms for oxymercuryation or ozonide decomposition to ketones, aldehydes, and/or carboxylic acids. You do NOT need to know mechanisms for cleavage of cyclic permanganate, periodate, or osmate esters. See 7.8.) |
| 10 | Calculate the oxidation state (or number) of atoms in organic molecules. |
| 11 | Classify reactions of organic molecules as oxidations, reductions, or neither. |
| 12 | All recommended and/or required problems and problems similar to them. |

**Cutoff for Exam 2 material.**

Things you should be able to do from Ch. 8:

|  |  |
| --- | --- |
| 1 | Name alkynes. Alkynes are lower in priority than alcohols but higher than alkyl halides, alkanes, and alkenes. |
| 2 | Predict geometry, hybridization, and bond angles for sp-hybridized carbons. |
| 3 | Draw a 3-D representation of -bonding in alkynes. |
| 4 | Synthesize alkynes by a double dehydrohalogenation of a dihalide. |
| 5 | \*Predict the products of the addition of HX, X2, H2/catalyst, H2O/H2SO4/Hg2+, BH3 followed by H2O2/HO-, H2/poisoned catalyst, Li or Na/NH3, KMnO4, or O3 to an alkyne. (If a poisoned catalyst, such as Lindlar palladium, is used in the hydrogenation, then a syn addition of one equivalent of H2, yielding a cis-alkene, will result.) |
| 6 | Provide a mechanism for a dissolving metal reduction of an alkyne to a trans-alkene using Na or Li or K and NH3. |
| 7 | Draw the products and provide a mechanism for the addition of HX across the pi bonds of an alkyne. |
| 8 | Provide a mechanism for the tautomerization of an enol to a ketone. |
| 9 | (Acid/base review) Recognize that terminal alkynes have a somewhat acidic H. Terminal alkynes can be deprotonated with a strong base (NaNH2). The alkyne anion will act as a nucleophile toward methyl and primary alkyl halides and as a base toward secondary and tertiary alkyl halides. |
| 10 | Draw products of the reaction between an alkyne anion and an alkyl halide. (See objective 9.) |
| 11 | \*Combine alkyne chemistry with reactions studied previously to accomplish synthetic transformations. (Specifically, a terminal alkyne can be deprotonated, allowed to react with a methyl or primary alkyl halide in an SN2 reaction, reduced to either a cis- or trans-alkene, and then any Ch. 7 reaction can be carried out.) |
| 12 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 10:

|  |  |
| --- | --- |
| 1 | Name alkyl halides or provide a structure if given the name. |
| 2 | Classify alkyl halides as methyl, primary, secondary, or tertiary. |
| 3 | Prepare alkyl halides from alkenes. |
| 4 | Rank radicals in order of stability. (Radical stability and carbocation stability follow the same trends. However, it is acceptable to propose methyl and primary radical intermediates.) |
| 5 | Predict the products of alkane halogenation. (Mechanism was discussed with Ch. 5 notes and is presented in the text in 10.3.) FYI, chlorinations are not very selective and you will convert any sp3C-H into a C-Cl bond. Over chlorination is often a problem. Brominations are much more selective and will proceed predominantly through the most stable radical. So, tertiary C-H’s are more likely to be converted to C-Br’s than are methyl, primary, or secondary C-H’s. Brominations can be successfully stopped at monobrominated products. |
| 6 | Provide products and a mechanism for the allylic halogenation of alkenes with NBS. |
| 7 | Provide products for reactions of alcohols with HX, SOCl2, or PBr3. |
| 8 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 11:

|  |  |
| --- | --- |
| 1 | Provide products and a mechanism for the conversion of alcohols to sulfonate esters, such as a tosylate. |
| 2 | Recognize that sulfonate esters can be used to convert an –OH to a better leaving group. |
| 3 | \*Predict products and show mechanisms of nucleophilic substitution reactions, including stereochemistry when necessary. |
| 4 | Determine if a given nucleophilic substitution proceeds predominantly by an SN1 or SN2 mechanism and explain how you know. |
| 5 | Provide electron-pushing mechanism and/or energy diagram for SN1 and SN2 reactions. |
| 6 | If given two reactions, predict which one will be faster by considering concentrations, leaving groups, steric effects, solvent effects, temperature, nucleophile strength (for SN2 reactions) and carbocation stability (for SN1 reactions.) |
| 7 | Understand why SN1 reactions follow first order reaction kinetics while SN2 reactions follow a second order reaction rate. |
| 8 | Provide a rate expression for a given reaction such as Rate = *k*[CH3Br][I-]. |
| 9 | \*Give products, complete electron-pushing mechanisms (SN1 or SN2), and/or energy diagrams for the conversion of alcohols to alkyl halides using hydrogen halides (HX). (Each step of the mechanism will go through a transition state and the rate-determining step must cross through the highest energy T.S.) |
| 10 | Use substitution reactions in an overall synthetic scheme. |
| 11 | Use Zaitsev’s rule to predict which alkene in a reaction will be formed as the major product of an elimination if multiple alkenes can be formed. |
| 12 | \*Predict the products of elimination reactions. Alcohols undergo dehydration reactions in acid. Alkyl halides undergo dehydrohalogenation reactions readily in base (E2) but can lose HX under neutral conditions if a stable carbocation intermediate can be formed (E1). |
| 13 | \*Provide a complete electron-pushing mechanism for dehydration and dehydrohalogenation reactions including all bonds formed, all bonds broken, and any by-products of the reaction. |
| 14 | Rank various alkyl halides in order of increasing reaction rate for a given mechanism (E1 or E2) by examining structure (1°, 2°, or 3°) and leaving group (F, Cl, Br, or I). |
| 15 | Understand why E1 reactions follow a first order reaction rate while E2 reactions follow a second order reaction rate. |
| 16 | Predict how changing the concentration of the alkyl halide (or alcohol) affects the rate of an elimination reaction. (For example, would doubling the concentration of a reagent double the reaction rate?) |
| 17 | Recognize that in E2 reactions, alkyl halides need to adopt a geometry in which H-C1 and C2-X orbitals are in the same plane prior to forming the C1=C2 -bond. Two geometries of the starting material are possible: syn-periplanar (higher energy) and anti-periplanar (lower energy). Anti-periplanar reactions are MUCH faster than syn-periplanar reactions. Predict products of reactions with this stereoelectronic requirement in mind. (See 11.11 and 11.12.) |
| 18 | Determine if a reaction will proceed predominately by substitution or elimination. |
| 19 | \*Predict the predominant mechanism for a given reaction as SN1, SN2, E1, or E2. |
| 20 | \*Design a multi-step organic synthesis of a given target molecule from a given starting material. You will most likely need to combine chemistry from Chs. 6, 7, 8 and 11. |
| 21 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 14 :

|  |  |
| --- | --- |
| 1 | Classify polyenes as isolated, conjugated, or cumulated. |
| 2 | Name polyenes. |
| 3 | Synthesize dienes by normal elimination reactions. |
| 4 | Use heats of hydrogenation to determine if polyenes are resonance stabilized. |
| 5 | Define HOMO and LUMO. |
| 6 | Provide a simple definition of a wavefunction () – an equation that describes the probability of finding an electron in space. |
| 7 | Draw -bonding and -antibonding molecular orbitals for ethene and 1,3-butadiene. You should be able to predict which orbitals will have electrons in them and rank the orbitals energetically as done in class for butadiene. |
| 8 | Draw resonance contributors for conjugated carbocations (and radicals) such as those that are allylic. (Resonance delocalization is always energetically favorable.) |
| 9 | Predict 1,2- and 1,4-addition products if given a conjugated diene and one equivalent of electrophile. You should also be able to provide a mechanism and a reaction energy diagram that explains the formation of both products. |
| 10 | Explain the difference between kinetically and thermodynamically controlled reactions. You should understand that at lower temperatures, reactants will irreversibly cross the lowest energy barrier. At higher temperature, reactants will reversibly cross energy barriers leading to the lowest energy product being formed in highest yield. |
| 11 | Predict products of the Diels-Alder reaction including the stereochemical features we discussed in lecture. You should also be able to provide a one-step mechanism for the Diels-Alder reaction. |
| 12 | Use the Diels-Alder reaction to synthesize a target molecule. |
| 13 | Predict what starting materials would be required to synthesize a given target molecule by the Diels-Alder reaction. |
| 14 | Define pericyclic reactions as opposed to cycloaddition reactions. (A Diels-Alder reaction is both pericyclic and a cycloaddition.) |
| 15 | If given the interacting molecular orbitals, predict whether a reaction is symmetry allowed or forbidden. |
| 16 | All recommended and/or required problems and problems similar to them. |

Molecular orbital theory is more mathematically correct than valence bond theory. We will use valence bond theory to model most of the chemistry we will see in organic. There are some reactions that are not explained well by valence bond theory alone. The conjugate addition reactions of Ch. 14 are best described by MO theory. If you continue taking chemistry courses, you will see more MO theory. I do not want you walking into an advanced chemistry class knowing absolutely nothing about MO theory. *What we have covered regarding molecular orbitals is meant to be an overview of things to come, not a central theme for an organic exam.*

**Cutoff for Exam 3 material.**

Things you should be able to do from Ch. 15:

|  |  |
| --- | --- |
| 1 | Name aromatic compounds (and their derivatives) by their IUPAC-accepted common names. You should know the structures of benzene, toluene, the xylenes, phenol, aniline, benzaldehyde, and benzoic acid. (See Table 15.1.) You should also know the structure of pyridine, pyrrole, and furan. (See pp. 528-30.) |
| 2 | Use ortho, meta, and para nomenclature to name disubstituted benzene rings. |
| 3 | Use heats of hydrogenation to calculate resonance energies. |
| 4 | Draw the resonance (Kekule) structures of benzene. |
| 5 | Classify hydrocarbons as aliphatic or aromatic. |
| 6 | Determine if a compound, including ions and compounds that contain heteroatoms, should display the special stabilization associated with aromaticity. (Huckel’s rule) |
| 7 | Combine reactions you have learned to provide a multi-step synthesis of a target molecule. |
| 8 | Predict the relative Bronsted-Lowry acid/base strengths with consideration of aromaticity. |
| 9 | Explain why cyclobutadiene and cyclooctatetraene are not aromatic. (They are actually antiaromatic with 4n -electrons.) |
| 10 | All recommended and/or required problems and problems similar to them. |

Things you should be able to do from Ch. 16:

|  |  |
| --- | --- |
| 1 | Show/explain mechanistically why aromatic compounds undergo substitution and not addition reactions. |
| 2 | \*Draw the products and mechanisms (including all electron-pushing arrows, intermediates, and by-products) of electrophilic aromatic substitution reactions. We have covered brominations, chlorinations, nitrations, Friedel-Crafts alkylations and acylations, and sulfonations. |
| 3 | Draw resonance contributors for arenium and acylium ions. |
| 4 | Predict the products of desulfonation reactions. |
| 5 | Predict if a substituent is ring-activating or ring-deactivating. |
| 6 | Predict relative rates of electrophilic aromatic substitution reactions due to the presence of ring activating and/or deactivating groups. |
| 7 | Provide a reaction energy diagram for an electrophilic aromatic substitution reaction. |
| 8 | Predict where an electrophile will add to a ring. You should be able to determine whether a substituent that is already on the ring directs incoming electrophiles o/p or m. You should also be able to predict where an electrophile will add if more than one substituent is already on the ring. |
| 9 | Determine where an electrophile will add to an aromatic ring that already has multiple substituents on the ring. |
| 10 | Synthesize compounds from benzene, any organic molecules of 3 carbons or less, and any inorganic reagents you need. You may be asked to add more than one substituent to the aromatic ring or to combine previous addition, substitution, and/or elimination reactions with the electrophilic aromatic substitution reactions. |
| 11 | Provide products of the reactions of KMnO4 or Na2Cr2O7/H2SO4 with alkyl benzenes. |
| 12 | Provide products and a mechanism for free-radical halogenation of benzylic carbons using either Br2/hv or NBS/benzoyl peroxide. |
| 13 | Provide products and/or reaction conditions for catalytic hydrogenation of aromatic rings. |
| 14 | Provide products and/or reaction conditions for catalytic hydrogenation of an aryl alkyl ketone. Recognize that the same reaction conditions also reduce a nitro group to an NH2. |
| 15 | All recommended and/or required problems and problems similar to them. |