CHEM 241 IN-CLASS PROJECT #3-Turn in one sheet per group.

NAMES

1. a. **Draw and name** the all alkenes which have the molecular formula $\text{C}_5\text{H}_{10}$. (hint: there are 6 total)

b. Which structures above would be considered 'geometric isomers' of each other.
2. Regarding the following 4 (#1-#4) reaction coordinate diagrams answer the following.

Which has the fastest rate? __________
Which has the slowest rate? __________
Which is the most exothermic (exergonic)? __________
Which is the most endothermic (Endergonic)? __________
Which has the smallest rate constant (k)? __________
Which has the largest ΔG° Value? __________
Which has the largest equilibrium constant (K)? __________
Which has the largest ΔG Value? __________
Part II In this section we will analyze the addition reaction of a double bond. The 2 step mechanism is shown below:

![Reaction Mechanism Diagram]

Stability of the carbocation intermediate

The first step of the reaction is the formation of two intermediates: $X^-$ and a carbocation (note the lack of an octet for the carbocation). The hydrogen of HX will add to the carbon of the C=C that will generate the most stable carbocation. The stability of the carbocation is determined by the number of carbons that surround the C+ atom. Adjacent carbons stabilize the carbocation by hyperconjugation (Bruce sec 4.2) leading to the result that $3^0$ is more stable than $2^0$ which is more stable than $1^0$.

![Stability Comparison Diagram]

Answer the following questions (1 and 2) regarding the reactions (A-D) shown below.

A
\[ \text{CH}_3\text{C} = \text{CCH}_2\text{CH}_3 + \text{HBr} \]

B
\[ \text{CH}_3\text{C} = \text{CCH}_2\text{CH}_3 + \text{HF} \]

C
\[ \text{CH}_3\text{C} = \text{CCH}_2\text{CH}_3 + \text{H}_2\text{O} \]

D
\[ \text{CH}_3\text{C} = \text{CCH}_2\text{CH}_3 + \text{HOCH}_3 \]

1.(a). Draw the most likely carbocation intermediate that would be formed each of the reactions A-D. If the carbocation intermediates are the same for all, draw it once and state 'same intermediate' for all. Also note if the carbocations are primary, secondary or tertiary.

1.(b). Assuming that the stability of the carbocation intermediate is the only factor that determines the rate of the reaction, rank reactions A-D in order of reactivity (fastest to slowest)? If they are all equal state 'all equal'.
2. (a). Draw the $X^-$ intermediate that would be formed for each of the reactions (A-D).

A:  
B:  
C:  
D:  

b). Assuming that the stability of $X^-$ intermediate determines the rate of the reaction, rank reactions A-D in order of reactivity (fastest to slowest). To determine the stability of $X^-$ use the same parameters that you used to determine the stability of a 'conjugate base' in the previous acid/base assignment. The table below should also give you some clues

<table>
<thead>
<tr>
<th>$X^-$</th>
<th>pKa</th>
<th>$HX \rightarrow H^+ + X^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Br$^-$</td>
<td>-2.2</td>
<td>$HBr \rightarrow H^+ + Br^-$</td>
</tr>
<tr>
<td>F$^-$</td>
<td>3.2</td>
<td>$HF \rightarrow H^+ + F^-$</td>
</tr>
<tr>
<td>HO$^-$</td>
<td>15.7</td>
<td>$H_2O \rightarrow H^+ + HO^-$</td>
</tr>
<tr>
<td>CH$_3$O$^-$</td>
<td>16</td>
<td>$CH_3OH \rightarrow H^+ + CH_3O^-$</td>
</tr>
</tbody>
</table>

3. From your answers given in questions #1 and #2 explain the experimental order of reactivity given for A-D shown below. (note: both intermediates are factors in determining the rate of reaction).

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Relative rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1000</td>
</tr>
<tr>
<td>B</td>
<td>1</td>
</tr>
<tr>
<td>C</td>
<td>0.0000001 (effectively no reaction)</td>
</tr>
<tr>
<td>D</td>
<td>0.0000001 (effectively no reaction)</td>
</tr>
</tbody>
</table>

4. Construct a statement regarding on how $X^-$ relates to the reactivity (rate of reaction) of an addition reaction.

5. What would be the result (regarding the rate of reaction) if we used $H_2O^+$ instead of water in reaction C? Elaborate on why the result would be different. Note: The pKa of $H_2O^+$ is -1.3

6. Suggest a way to increase the rate of reaction D?
7. Draw the 3 reaction coordinate diagrams would correspond to reactions A, B and C. Be sure to show the relative value of the intermediates and $\Delta G^\circ$ of activation. Assume all reactions are exothermic.

8. Draw a mechanism to explain the unexpected outcome of the reaction shown below. Note that this reaction is under acidic conditions which means that no negatively charged species (-) can be formed.