

WORKSHOP 5

Alkene Structures

1. Three dicarboxylic acids, $C_2H_2(CO_2H)_2$, **I**, **J**, and **K**, are catalytically hydrogenated (react with H_2 in the presence of a catalyst) to give dicarboxylic acids with formulas of $C_2H_4(CO_2H)_2$. Hydrogenation of both **I** and **J** gives the same dicarboxylic acid **L**. Compound **K** hydrogenates to form compound **M**. Give structures for compounds **I-M**. **Explain your reasoning.**

OBSERVATION

DEDUCTION

2. Consider the data about **C-H** bonds in the following table. Discuss the variations in bond length, bond dissociation energy, IR stretching frequency and pK_a in terms of the observed geometries and concepts relating structure and bonding.

Molecule	$\angle CCH$	Bond Length Å	BDE in kJ/mol	BDE in kcal/mol	IR stretch, cm^{-1}	pK_a
Ethane	109.6	1.10	420	100	2850-2960	62
Ethylene	121.7	1.08	444	106	3020-3100	45
Acetylene	180	1.06	552	132	3300	26

3. Draw an atomic orbital model for $CH_2=C=CH_2$. Consider first the geometry at each carbon and select the appropriate hybridization. Label the orbitals used and show all valence electrons. The geometry should be clear from your drawing. Draw a dash/wedge structure for it.

Compare the geometry of this molecule with that of a typical alkene.

4. Write a detailed stepwise mechanism for the transformation shown below. Identify each species in the mechanism as a Lewis acid or Lewis base and use curved arrows to show the movement of electron pairs. Construct a plot that describes the energy of the system as a function of the progress of the reaction (reaction energy diagram). On your diagram, clearly label the positions of the reactants, any intermediate(s), and the product. Also, specify the energy difference that corresponds to the ΔG° for the overall reaction and the energy difference that corresponds to ΔG^\ddagger for each step. Explain (in words) what is happening as the system makes its way from reactants to products.

