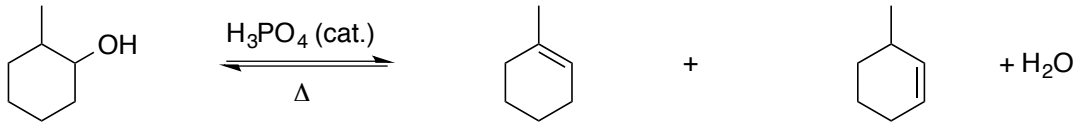
CHEM 8L

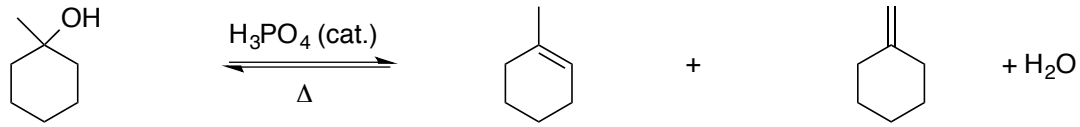
Lab Calculations

****Work the problems below on a separate sheet of paper. Show your work with units on every value using dimensional analysis.**

1.The acid-promoted dehydration of alcohols affords a mixture of two alkene isomers, along with water. Next week, students will carry out this reaction using with 750 μL of 1-methylcyclohexanol (density = 0.919 g/mL) or 2-methylcyclohexanol (density = 0.93 g/mL) and 225 μL of a concentrated solution of phosphoric acid (85% w/w, sol'n density = 1.685 g/mL). Note: "w/w" = weight per weight, which translates into 85 g of pure H_3PO_4 per 100 g of solution.



2-Methylcyclohexanol **1-Methylcyclohexene** **3-Methylcyclohexene**



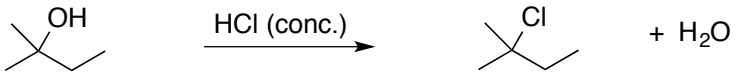
1-Methylcyclohexanol **1-Methylcyclohexene** **Methylenecyclohexane**

(a) Convert the amounts of 1-methylcyclohexanol, 2-methylcyclohexanol, and phosphoric acid into mmols. Calculate molar masses using the structures above.

(b) What is the limiting reagent in the reaction of 2-methylcyclohexanol with phosphoric acid? What is the theoretical yield (in mg) of the mixture of alkenes in this reaction (both alkene products have the same molecular mass)?

(c) What is the limiting reagent in the reaction of 1-methylcyclohexanol with phosphoric acid? What is the theoretical yield in this reaction?

2.Unimolecular substitution (S_N1) reactions are favored when tertiary substrates, such as 2-methyl-2-butanol, are reacted with a good nucleophile (Cl^-) under protic (acidic) conditions. The reaction below will be completed during the lab practical. Students will combine 1.00 mL of 2-methyl-2-butanol (density = 0.805 g/mL) with 2.5 mL of a concentrated solution of hydrochloric acid (37% w/w, sol'n density = 1.2 g/mL).



***t*-Pentanol**
(2-methyl-2-butanol)

***t*-Pentyl chloride**
(2-chloro-2-methyl-butane)

(a) Convert the amounts of 2-methyl-2-butanol and HCl into mmols. Calculate molar masses using the structures above.

(b) What is the limiting reagent in this reaction? What is the theoretical yield (in mg) of the chlorinated product (2-chloro-2-methylbutane)?

CHEM 8L

IR Problems

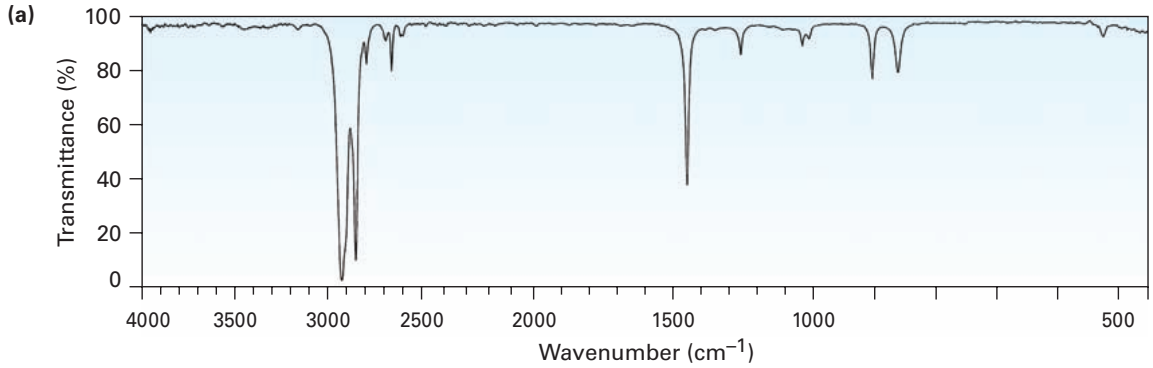
1. How could you use IR spectroscopy to distinguish between the following pairs of isomers:
a) CH_3CH_2OH and CH_3OCH_3 **b)** cyclohexane and 1-hexene
c) $CH_3CH_2CO_2H$ and $HOCH_2CH_2CHO$ (an aldehyde)

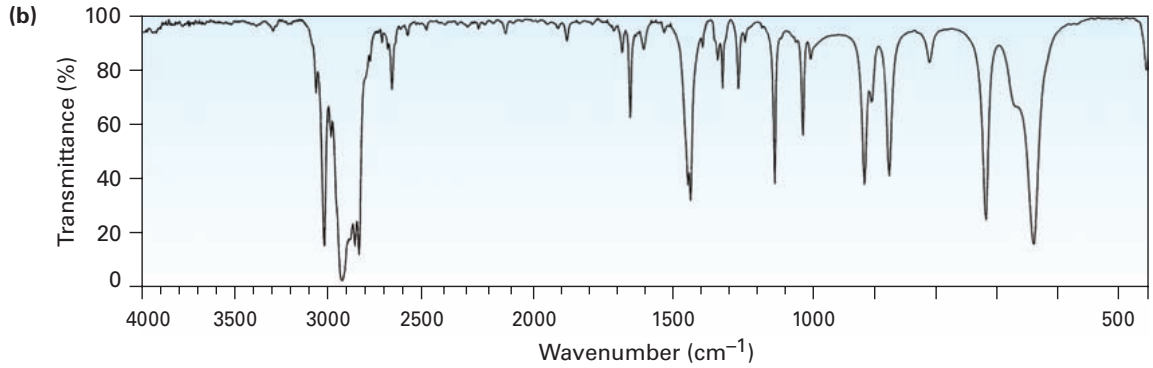
2. What functional groups might the following molecules contain?
a) A compound with a strong absorption at 1710 cm^{-1}
b) A compound with a strong absorption at 1540 cm^{-1}
c) A compound with strong absorptions at 1720 cm^{-1} and 2500-3100 cm^{-1}

3. Acetone (CH_3COCH_3) and 2-propen-1-ol ($H_2C{=}CHCH_2OH$) are isomers. How could you distinguish them by IR spectroscopy?

4. Propose structures for compounds that meet the following descriptions:
a) C_5H_8, with IR absorptions at 3300 and 2150 cm^{-1}
b) C_4H_8O, with a strong IR absorption at 3400 cm^{-1}

5. Two IR spectra are below. One is for cyclohexane and the other for cyclohexene. Identify them and explain your answer.





IR problems reproduced from McMurry, J. "Organic Chemistry, 8th edition."