

Name: _____

Sec. _____

Chem 226/ Dr. Rusay

Synthesis of Acetate Esters Prelab
Odor, Functions & Structures

As you have experienced in previous experiments, certain functions and stereochemistries correlate fairly well with a particular smell. In the perfume industry oxygen containing functions predominate in the chemistry of their products' "notes".

Refer to the following required reading that is on reserve in the DVC library under Dr. R's name for a complete review and answers to the post-lab questions.

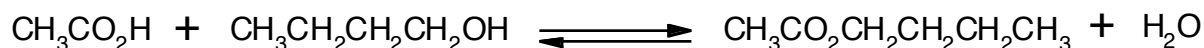
"Structure-Odor Relationships", Karen J. Rossiter, Chem. Rev., 96, 3201-3240, 1996
(Library Reserve) *Reading: pp. 3201-04, 3206, 3214, 3216, 3221-23.*

In Part I you will synthesize and analyze a molecule with one such function, an ester.

In Part II you will use Infrared spectroscopy to analyze various molecules that have different functions, which contain oxygen, including your synthetic ester product.

Esters are generally "fruity" in their smell. They are prepared from a carboxylic acid or one of its derivatives and an alcohol. Neither of the starting materials smell as the ester that is formed. Esters are named after their parent carboxylic acid and alcohol.

For the reaction of n-butanol (n-butyl alcohol) with acetic acid (vinegar), the product that is produced, butyl acetate, smells "fruity".



Note the way that the product is written. If it were written as $\text{CH}_3\text{O}_2\text{CCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$, it would no longer be the same ester. It would be methyl pentanoate.

- Five different esters will be synthesized in the entire class. You have randomly been assigned one of them. The smells include: orange, pear, banana, apple, and peach. One additional ester is included in the post lab: "juicy fruit" as in the gum. In the respective blocks on the left match the ester's name with the letter of the appropriate smell from the choices on the right.

<i>Ester's Smell</i>	<i>Ester's Name</i>	<i>Smell</i>
	propyl acetate	A) pear
	benzyl acetate	B) apple
	isopentyl acetate	C) peach
	isopentenyl acetate	D) banana
	isobutyl acetate	E) orange
	octyl acetate	F) juicy fruit

2. Draw a line or condensed structure for each of the esters, and complete the table below.

	<i>Ester Structure</i>	<i>Molecular Formula</i>	<i>Molar Mass</i>	<i>b.p.</i>
<i>pear</i>				
<i>apple</i>				
<i>peach</i>				
<i>banana</i>				
<i>orange</i>				

3. The five different esters will be synthesized from five different alcohols. Draw a line or condensed structure for each of the respective alcohols, and complete the table below.

	<i>Alcohol Structure</i>	<i>Molecular Formula</i>	<i>Molar Mass</i>	<i>density</i>	<i>b.p.</i>
<i>pear</i>					
<i>apple</i>					
<i>peach</i>					
<i>banana</i>					
<i>orange</i>					

4. For the synthesis of your assigned ester calculate the quantities of glacial acetic acid, alcohol, and sulfuric acid needed for the reaction based on producing a theoretical quantity 7.5 g of ester (assume 100% yield.) Use 2x-3x the molar equivalent of glacial acetic acid compared to the alcohol.