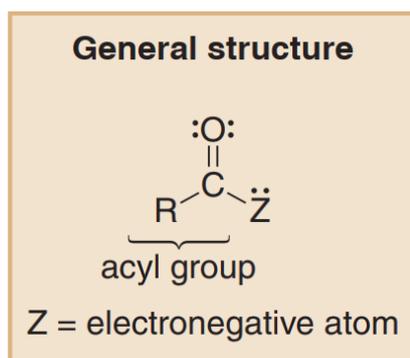


كلية التربية للعلوم الصرفة	الكلية
قسم الكيمياء	القسم
Organic chemistry	المادة باللغة الانجليزية
الكيمياء العضوية	المادة باللغة العربية
المرحلة الثانية	المرحلة الدراسية
د. عمر جمال مهدي العسافي	اسم التدريسي
Ester	عنوان المحاضرة باللغة الانجليزية
الاستر	عنوان المحاضرة باللغة العربية
الثانية عشر	رقم المحاضرة
<i>Organic Chemistry</i> 6 <sup>ed</sup> , William H. Brown, Christopher S. Foote, Brent L. Iverson, Eric V. Anslyn, Bruce M. Novak, 2012	المصادر والمراجع
<i>Organic Chemistry</i> 3 <sup>ed</sup> , Janice Gorzynski Smith, 2011	
<i>Organic Chemistry</i> '' by Jonathan Clayden, Nick Greeves, and Stuart Warren	

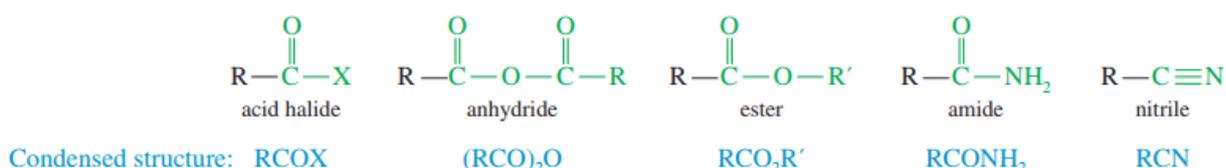


## 1. Introduction

Carbonyl compounds bonded to an electronegative atom called an acyl group. These include carboxylic acids and their derivatives such as acid esters,.



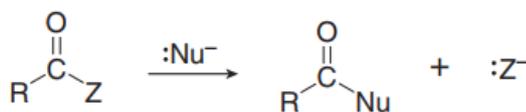
Carboxylic acid derivatives are defined as compounds with functional groups that can be converted to carboxylic acids by a simple acidic or basic hydrolysis.



All of these compounds contain an acyl group bonded to an electronegative atom **Z** that can serve as a leaving group. As a result, these compounds undergo nucleophilic acyl substitution.

Recall that aldehydes and ketones do not undergo nucleophilic substitution because they have no leaving group on the carbonyl carbon.

**Nucleophilic substitution**

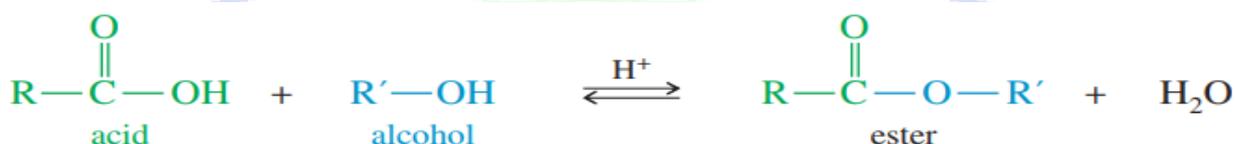


**Nu replaces Z.**

## 2-Nomenclature

The names of carboxylic acid derivatives are formed from the names of the parent carboxylic acids discussed in section previous. Keep in mind that the common names formic acid, acetic acid, and benzoic acid are virtually always used for the parent acid, so these common parent names are used for their derivatives as well.

### ➤ Naming an Ester—RCOOR'

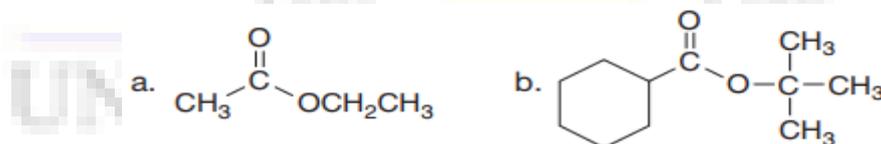


An ester has two parts to its structure, each of which must be named: an **acyl group** (RCO –) and an **alkyl group** (designated as R') bonded to an oxygen atom.

- ❖ In the IUPAC system, esters are identified by the suffix –ate.
- ❖ Esters are often written as RCOOR', where the alkyl group (R') is written last. When an ester is named, however, the R' group appears first in the name.

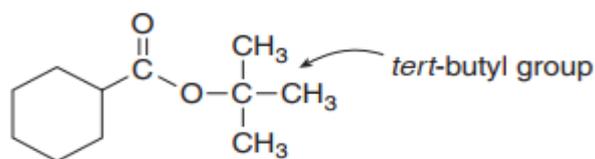
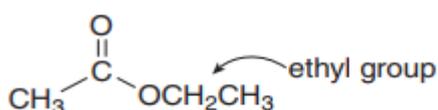
### HOW TO Name an Ester (RCO2R') Using the IUPAC System?

Example Give a systematic name for each ester:



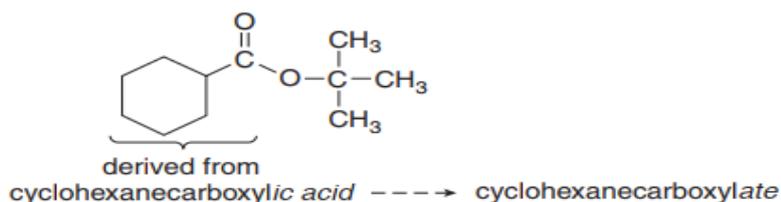
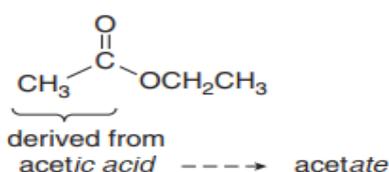
### Step1:- Name the R' group bonded to the oxygen atom as an alkyl group.

- The name of the alkyl group, ending in the suffix -yl, becomes the first part of the ester name.



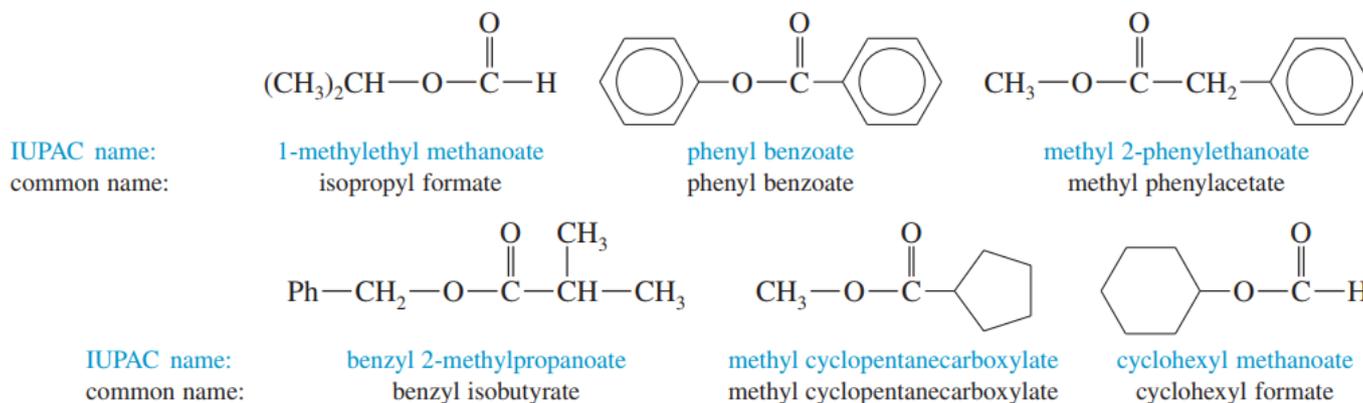
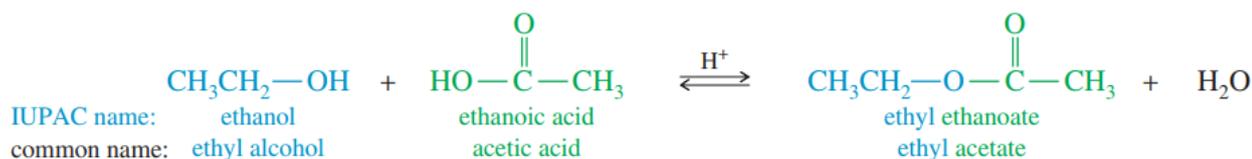
**Step [2] Name the acyl group (RCO – ) by changing the -ic acid ending of the parent carboxylic acid to the suffix -ate**

- The name of the acyl group becomes the second part of the name.

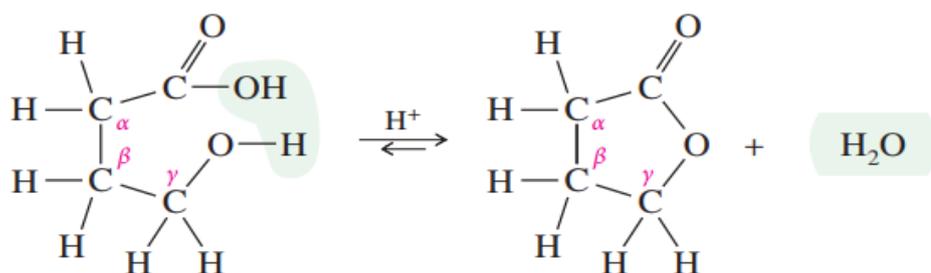


**Answer: ethyl acetate**

**Answer: tert-butyl cyclohexanecarboxylate**

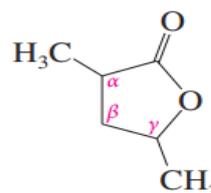
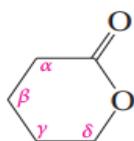


**Lactones** Cyclic esters are called **lactones**. A lactone is formed from an open-chain hydroxy acid in which the hydroxy group has reacted with the acid group to form an ester.

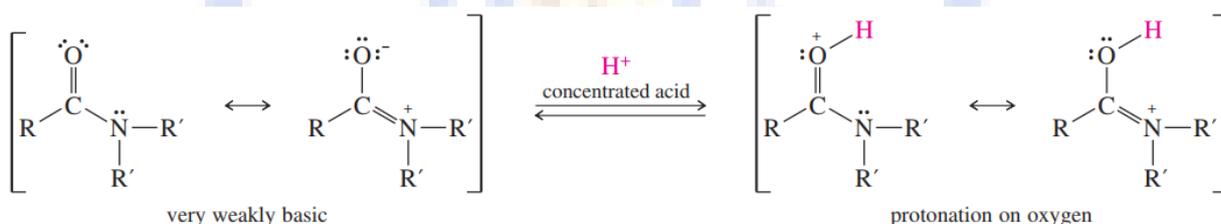


IUPAC name: 4-hydroxybutanoic acid      4-hydroxybutanoic acid lactone  
 common name:  $\gamma$ -hydroxybutyric acid       $\gamma$ -butyrolactone

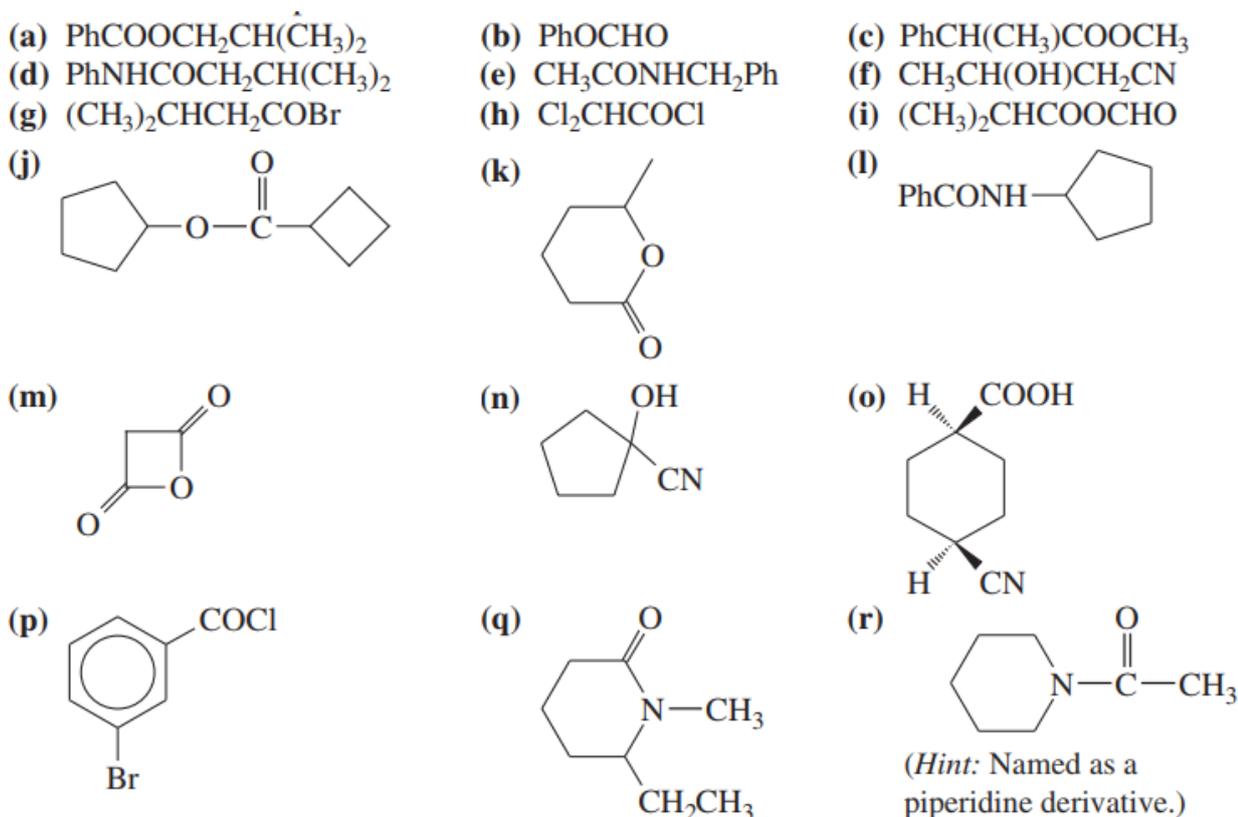
The IUPAC names of lactones are derived by adding the term lactone at the end of the name of the parent acid. The common names of lactones, used more often than IUPAC names, are formed by changing the *-ic acid* ending of the hydroxy acid to *-olactone*. A Greek letter designates the carbon atom that bears the hydroxy group to close the ring. Substituents are named just as they are on the parent acid.



IUPAC name: 5-hydroxypentanoic acid lactone      4-hydroxy-2-methylpentanoic acid lactone  
 common name:  $\delta$ -valerolactone       $\alpha$ -methyl- $\gamma$ -valerolactone



**PROBLEM :** Name the following carboxylic acid derivatives, giving both a common name and an IUPAC name where possible.



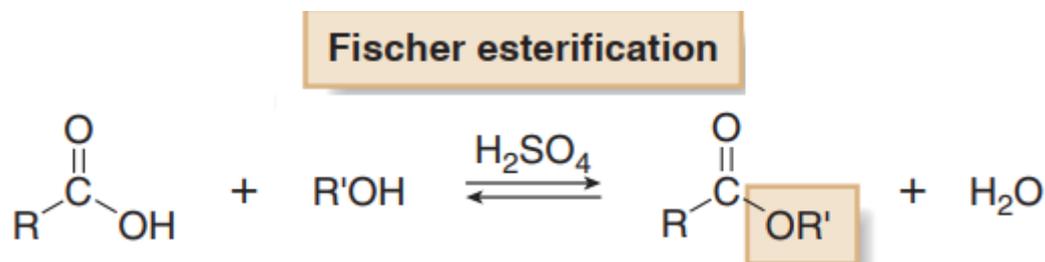
**Solution:**

(Hint: Named as a piperidine derivative.)

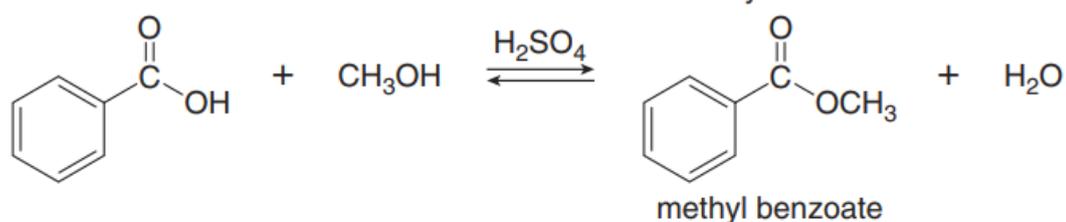
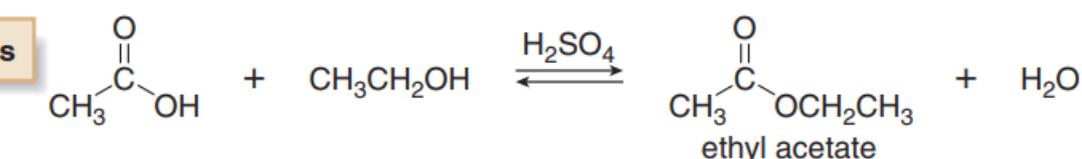
- isobutyl benzoate (both IUPAC and common)
- phenyl methanoate; phenyl formate
- methyl 2-phenylpropanoate; methyl  $\alpha$ -phenylpropionate
- 3-methyl-*N*-phenylbutanamide;  $\beta$ -methylbutyranilide
- N*-benzylethanamide; *N*-benzylacetamide
- 3-hydroxybutanenitrile;  $\beta$ -hydroxybutyronitrile
- 3-methylbutanoyl bromide; isovaleryl bromide
- dichloroethanoyl chloride; dichloroacetyl chloride
- methanoic 2-methylpropanoic anhydride; formic isobutyric anhydride
- cyclopentyl cyclobutanecarboxylate (both IUPAC and common)
- 5-hydroxyhexanoic acid lactone;  $\delta$ -caprolactone
- N*-cyclopentylbenzamide (both IUPAC and common)
- propanedioic anhydride; malonic anhydride
- 1-hydroxycyclopentanecarbonitrile; cyclopentanone cyanohydrin
- cis*-4-cyanocyclohexanecarboxylic acid; no common name
- 3-bromobenzoyl chloride; *m*-bromobenzoyl chloride
- 5-(*N*-methylamino)heptanoic acid lactam; no common name
- N*-ethanoylpiperidine; *N*-acetylpiperidine

### 3. Conversion of RCOOH to RCOOR'

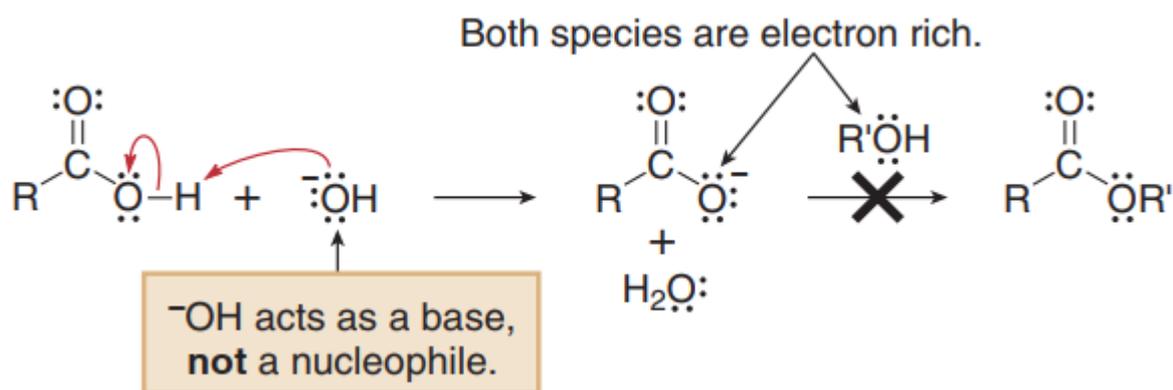
Treatment of a carboxylic acid with an alcohol in the presence of an acid catalyst forms an ester. This reaction is called a Fischer esterification.



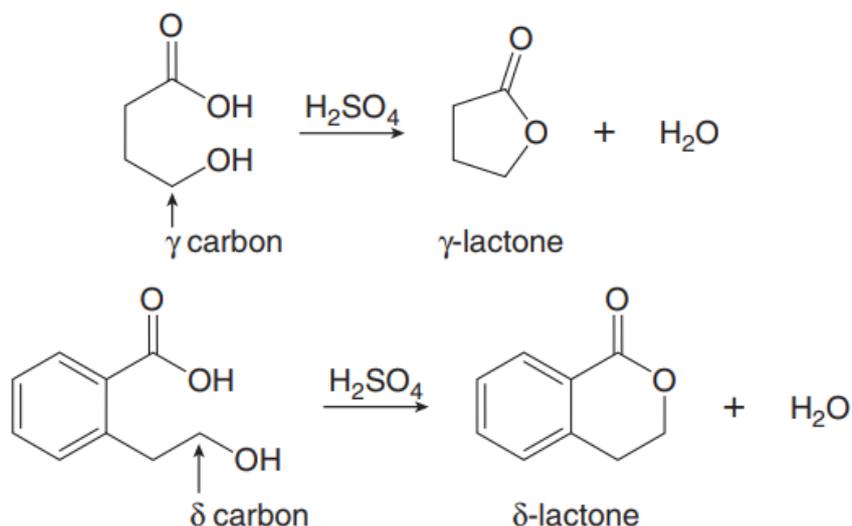
#### Examples



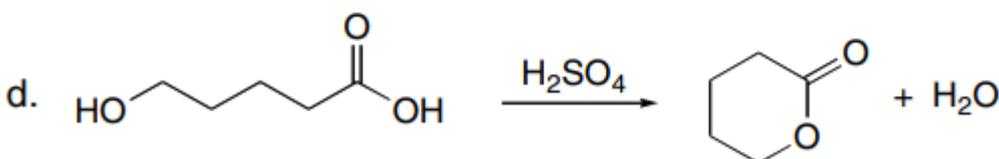
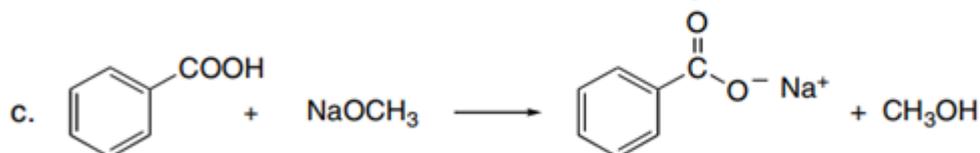
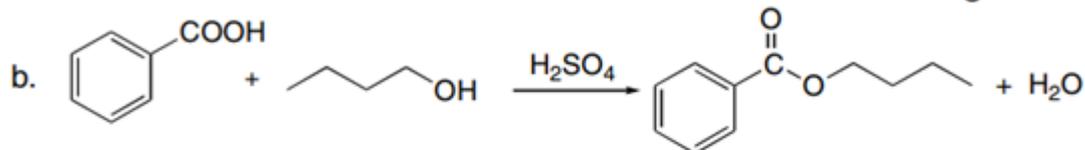
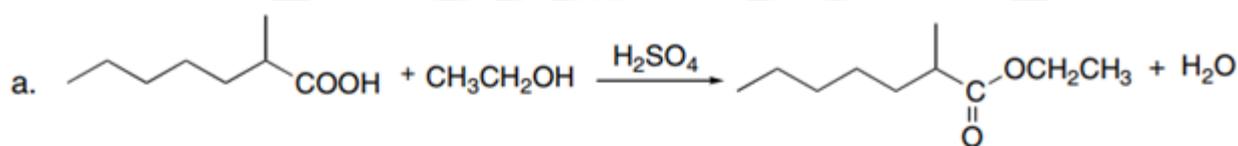
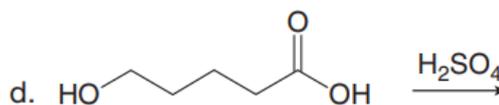
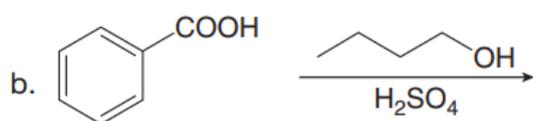
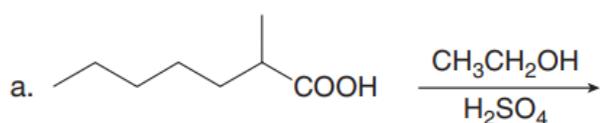
Esterification of a carboxylic acid occurs in the presence of acid but not in the presence of base. Base removes a proton from the carboxylic acid, forming a carboxylate anion, which does not react with an electron-rich nucleophile.



Intramolecular esterification of  $\gamma$ - and  $\delta$ -hydroxy carboxylic acids forms five- and six-membered lactones.



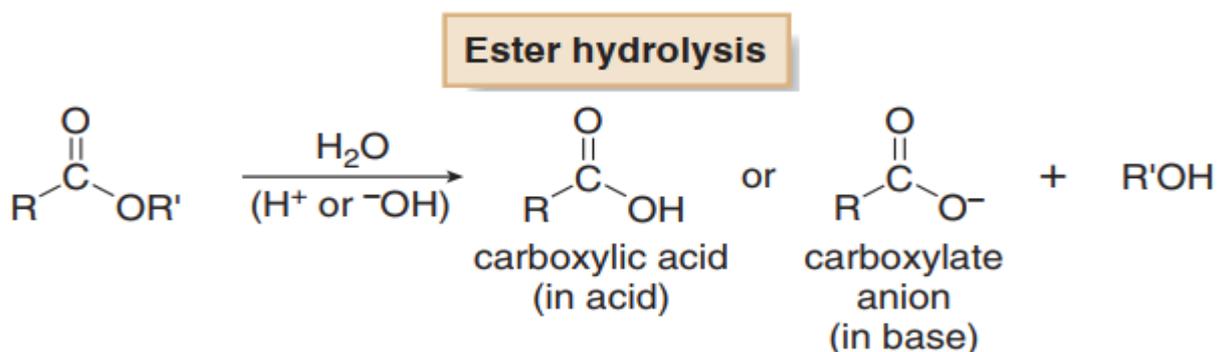
**Problem:** Draw the products of each reaction.



## 4. Reactions of Esters

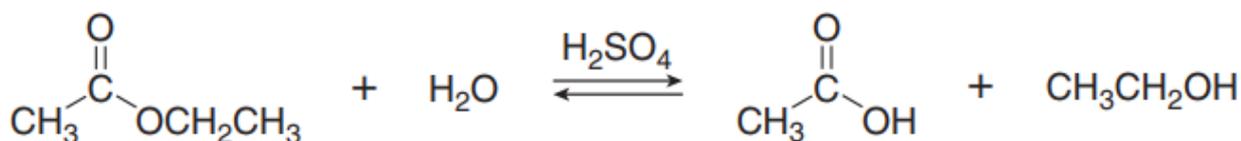
Esters can be converted into carboxylic acids and amides.

- Esters are hydrolyzed with water in the presence of either acid or base to form carboxylic acids or carboxylate anions.



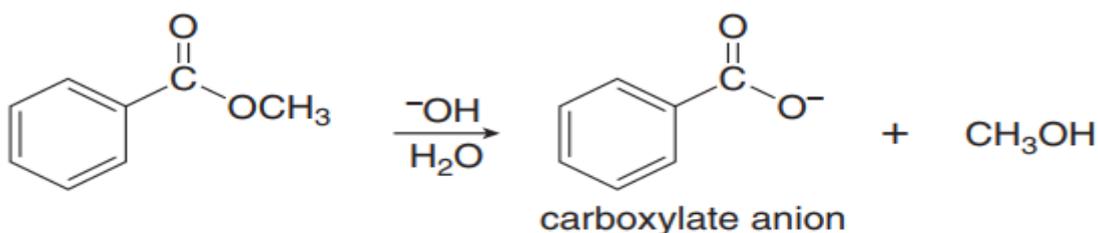
### ❖ Ester Hydrolysis in Aqueous Acid

The hydrolysis of esters in aqueous acid is a reversible equilibrium reaction that is driven to the right by using a large excess of water.



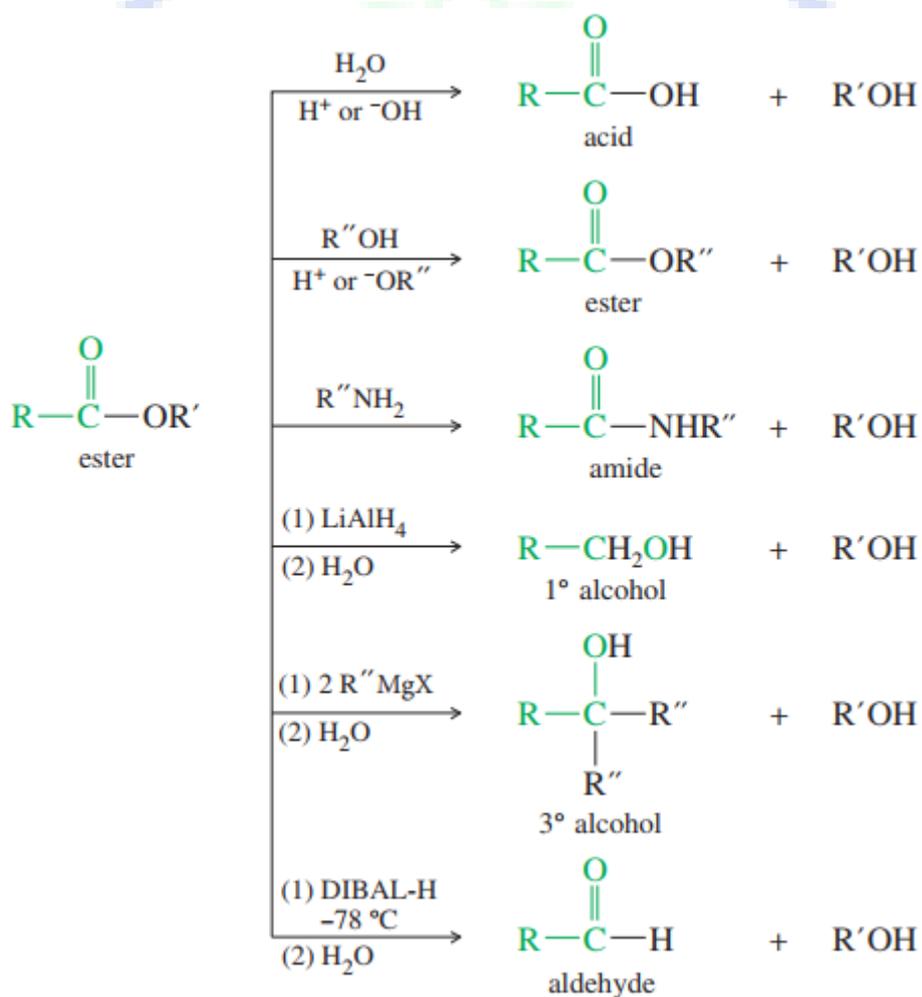
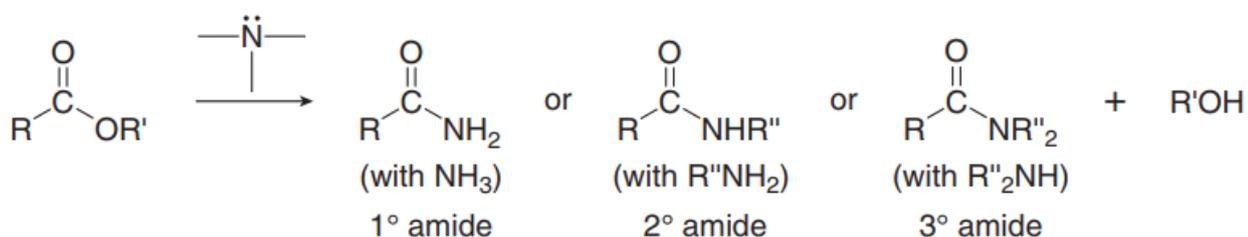
### ❖ Ester Hydrolysis in Aqueous Base

Esters are hydrolyzed in aqueous base to form carboxylate anions. Basic hydrolysis of an ester is called saponification.



Esters react with  $\text{NH}_3$  and amines to form  $1^\circ$ ,  $2^\circ$ , or  $3^\circ$  amides.

**Reaction with nitrogen nucleophiles**



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