Organic Molecules Tutorial

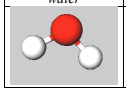
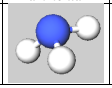
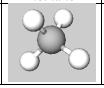
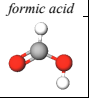
Functional Groups

Dr. Ron Rusay

Functional Groups & Amino Acids

Organic Molecules & Functional Groups

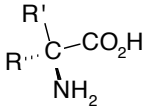
The following simple molecules: water, ammonia, methane, formaldehyde and formic acid can be used as "lego-like" building blocks to construct the vast majority of organic and biological molecules. Simply replace a hydrogen from each of any two molecules with a bond to the central atom, and if joining three molecules replace 4 hydrogens with 2 bonds.

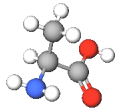
water	*ammonia*	*methane*	*formaldehyde*	*formic acid*
				

Name	**General Formula**
Alcohols	R−OH
Ethers	R−O−R′
Amines	$R-NH_2$
Carboxylic Acids	
Aldehydes	
Ketones	
Carboxylic Acids	
Esters	
Amides	

Chem 108 / Dr. Rusay

20 Amino Acids found in Proteins of Living Organisms

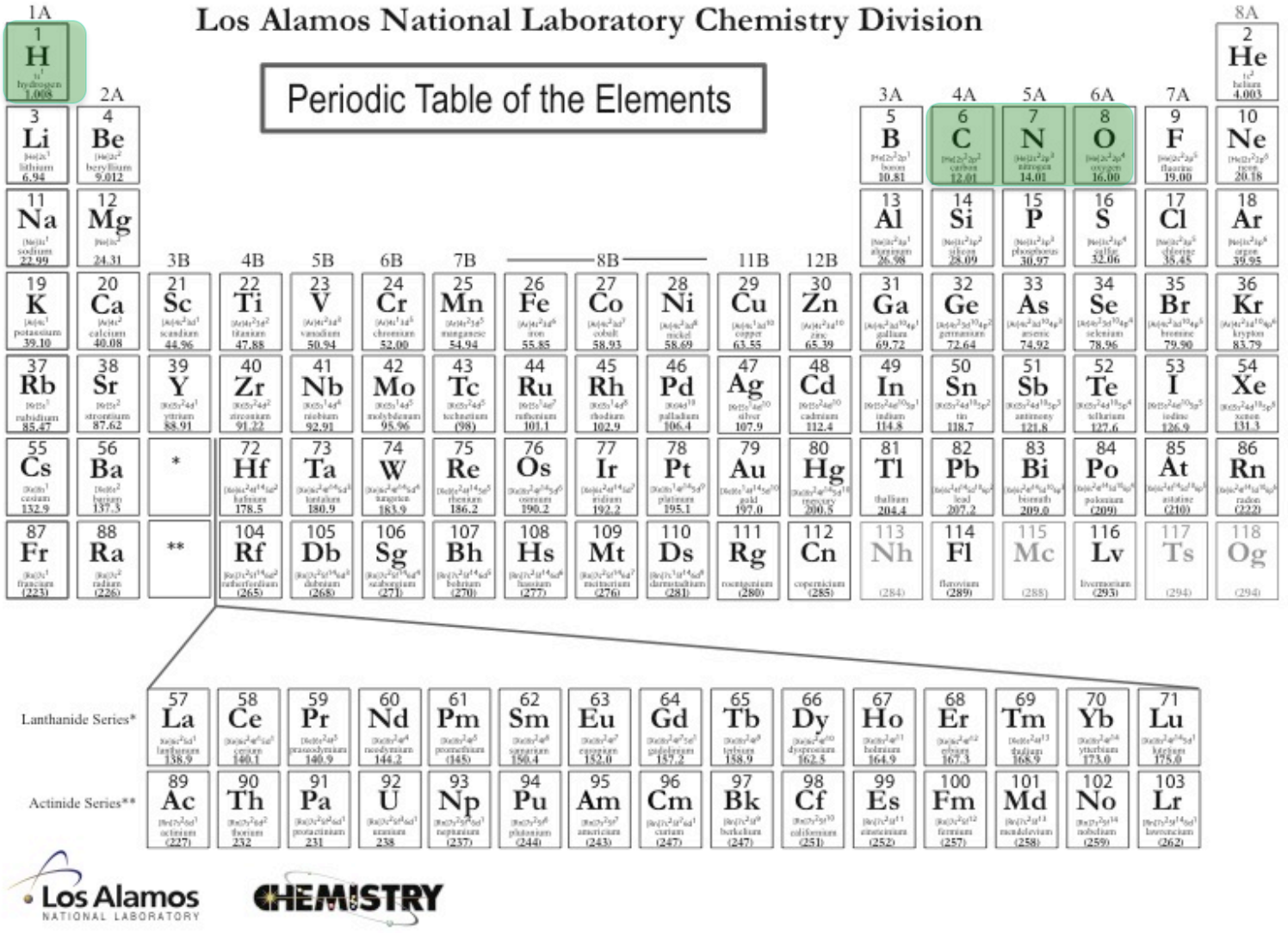




https://chem.libretexts.org/LibreTexts/Diablo_Valley_College/DVC_Chem_106%3A_Rusay/Amino_Acids

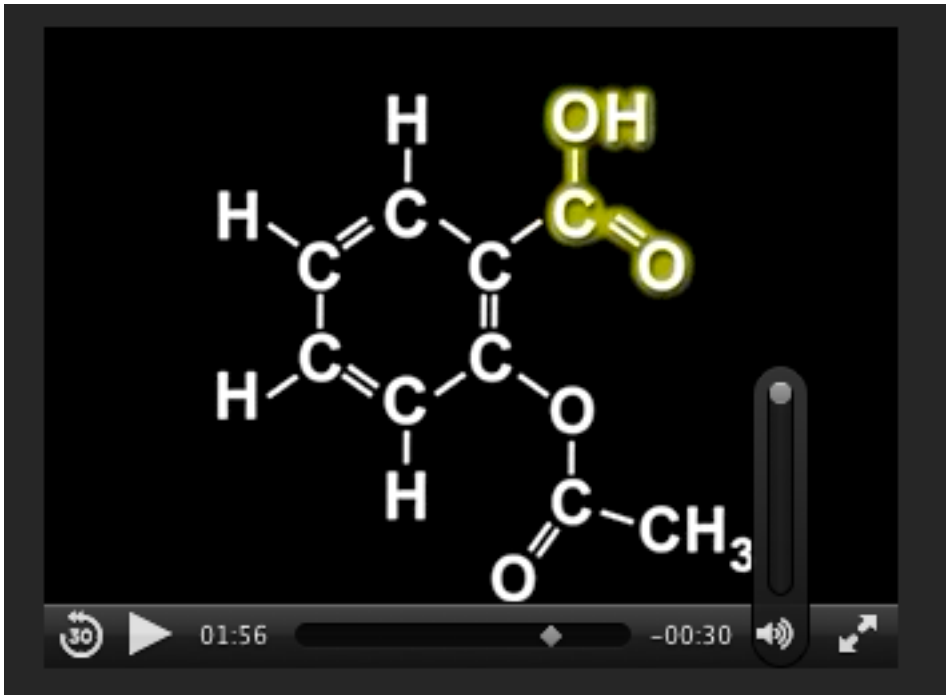
Name	I	II	R-	R'-	Rasmol Color	Function & Class
Alanine	Ala	A	H-	CH_3-	dark gray	Aliphatic Hydrophobic
Arginine	Arg	R	H-		blue	Basic Hydrophilic
Asparagine	Asn	N	H-		cyan	Amide Highly Hydrophilic
Aspartate	Asp	D	H-		bright red	Acidic Hydrophilic
Cysteine	Cys	C	H-	$-CH_2SH$	yellow	Sulphur Containing Hydrophobic
Glutamine	Gln	Q	H-		cyan	Amide Highly Hydrophilic
Glutamate	Glu	E	H-		bright red	Acidic Hydrophilic
Glycine	Gly	G	H-	H-	light gray	Aliphatic Hydrophobic
Histidine	His	H	H-		pale blue	Basic Hydrophilic
Isoleucine	Ile	I	H-		green	Aliphatic Hydrophobic
Leucine	Leu	L	H-		green	Aliphatic Hydrophobic

Elemental building blocks for all organic molecules



Synthesis of a Non-steroid anti-inflammatory drug

Aspirin



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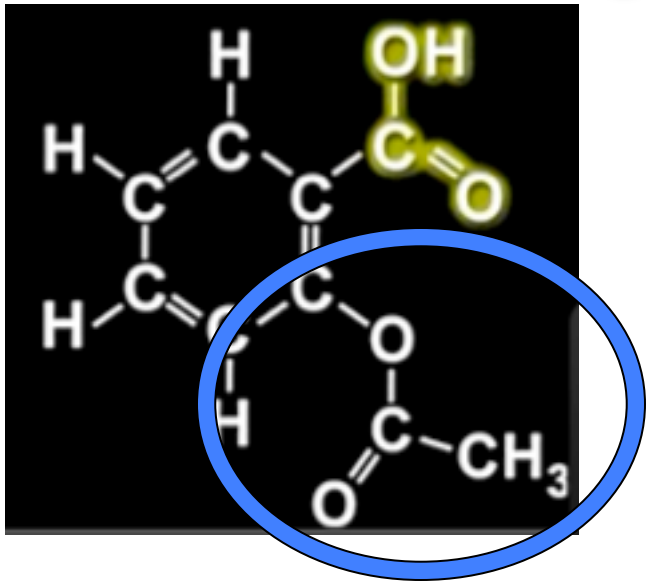
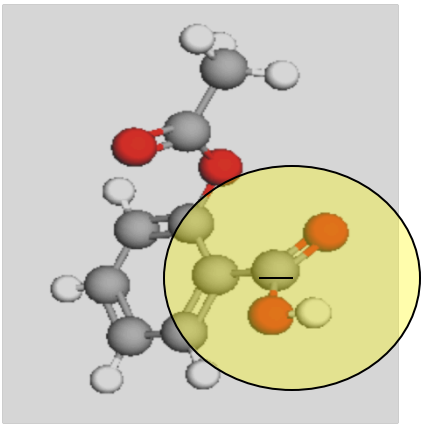
QUESTION

#1





One of aspirin's functions, an ester, is circled in blue. What is the highlighted yellow function?:

A.Alcohol

B.Ether

C.Ketone

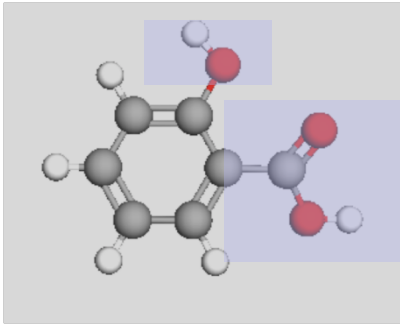
D.Aldehyde

E.Carboxylic Acid

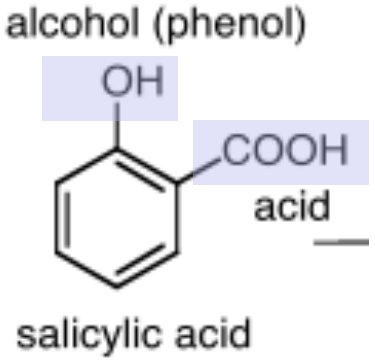
http://chemconnections.org/general/chem108/o-chem%20tutorial/Screen%20Shot%202018-12-07%20at%203.49.36%20PM.png

Salicylic Acid

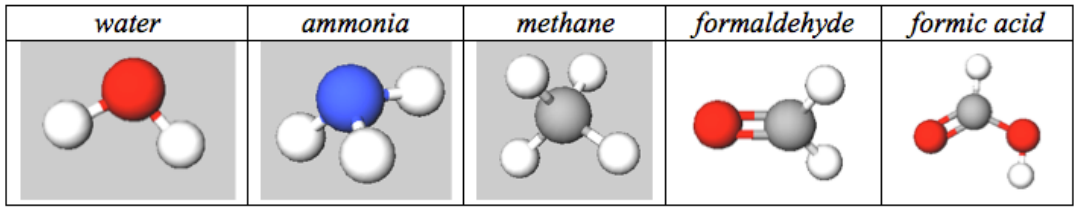
Common Functional Groups



Name	General Formula
Alcohols	R–OH
Ethers	
Amines	
Carboxylic Acids	R-C(=O)-OH

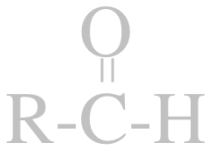
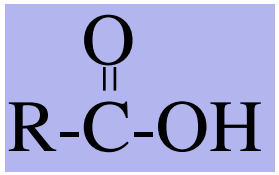
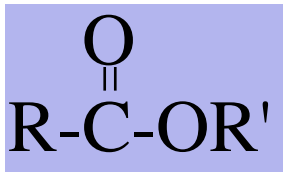
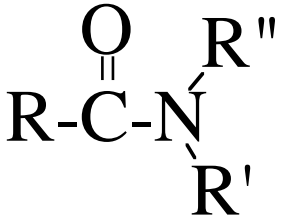


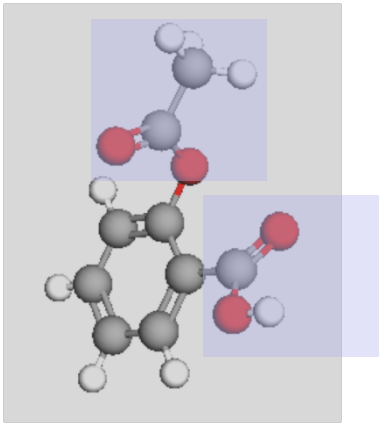
salicylic acid

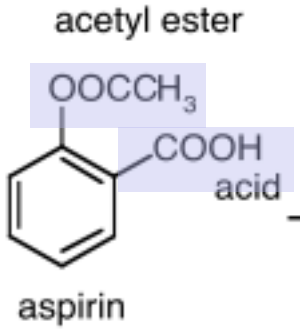


Aspirin

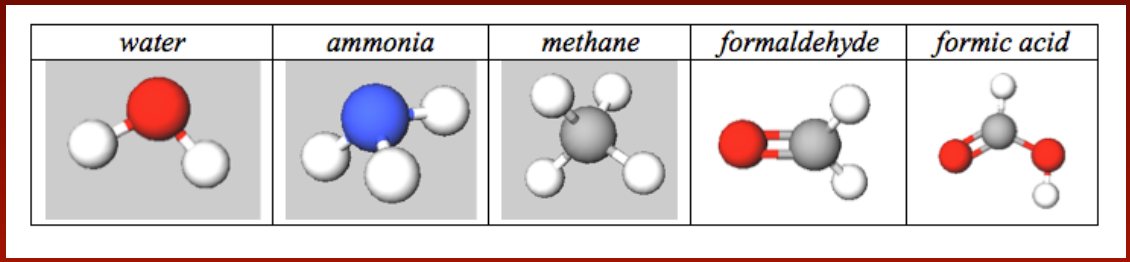
Common Functional Groups

Name	General Formula
Aldehydes	
Ketones	
Carboxylic Acids	
Esters	
Amides	



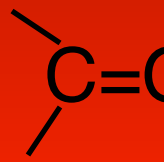


Organic Molecules



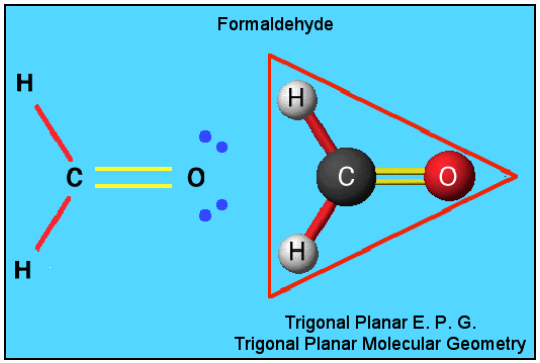
Shapes, Functions & Structural Analogies

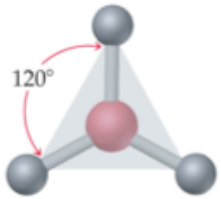
Water, Ammonia, Methane

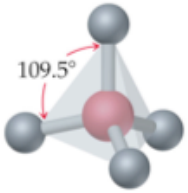
Plus  C=O “carbonyls”

Molecular Models for C, H, N, O

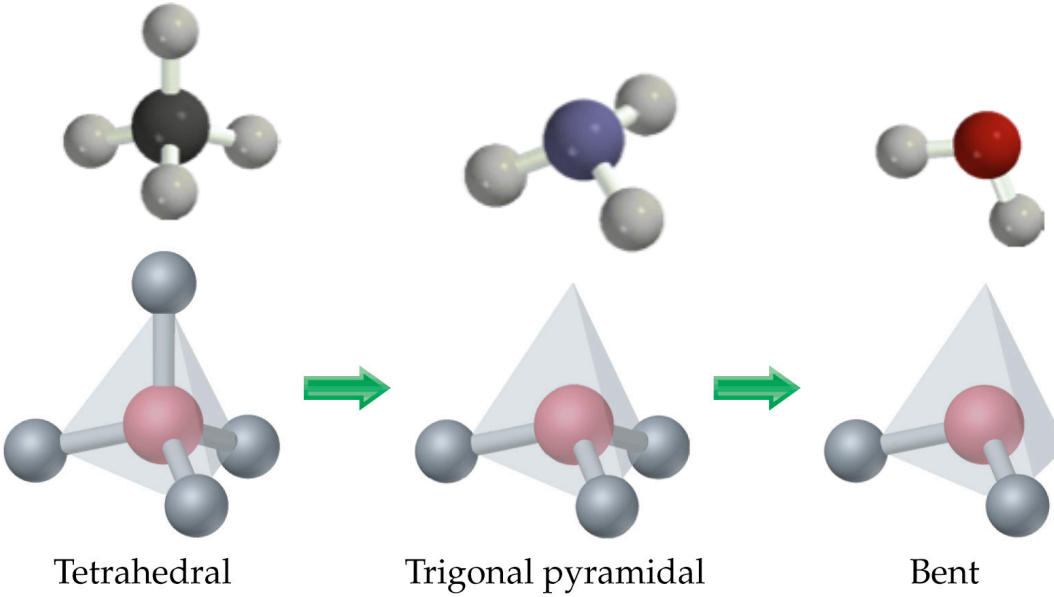
Fundamental repeating shapes found in every biological molecule







C =black
H = gray
N = blue
O = oxygen



pink = generic atom

Representing Organic Molecules

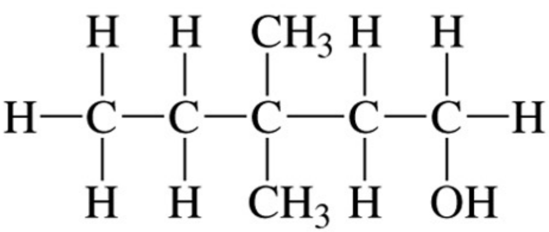
http://chemconnections.org/general/movies/Representations.MOV

Representing Organic Molecules

Common Formulas & Drawings

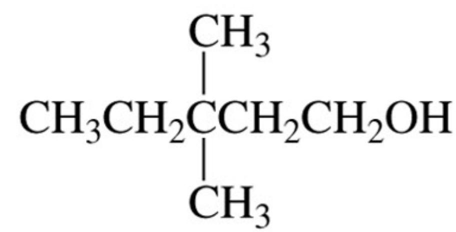
Molecular formula: $C_7H_{16}O$

Empirical Formula: $C_7H_{16}O$

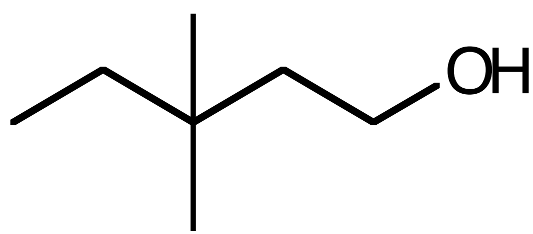


Condensed Structure:

$CH_3CH_2C(CH_3)_2CH_2CH_2OH$ or



Bond-Line Structure:

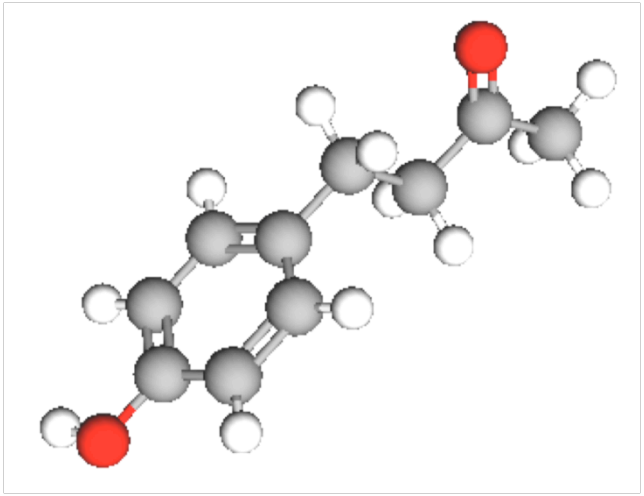


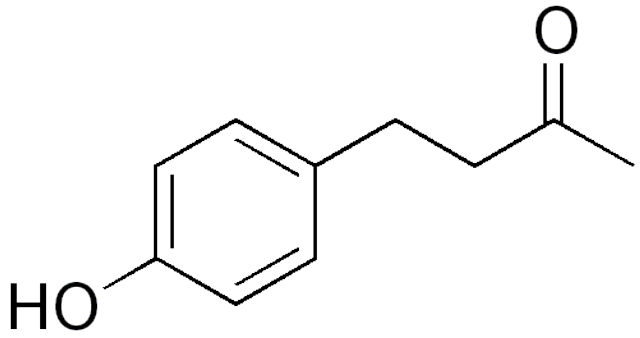
QUESTION

#2

A compound that smells like fresh raspberries, the following structure, $C_?H_?O_?$, matches its calculated molar mass which is 164 g/mol.

A) TRUE
B) FALSE





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Organic Molecules

Common Functional Groups

Name	General Formula
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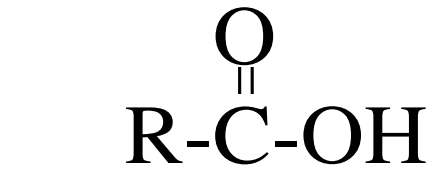
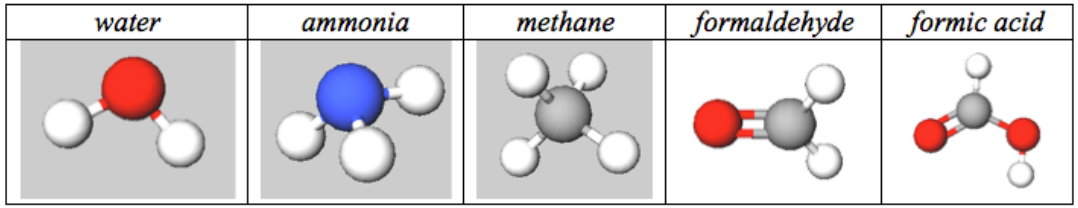
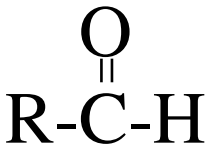
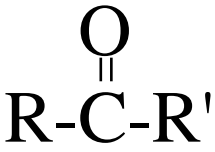
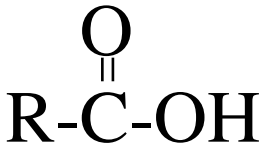
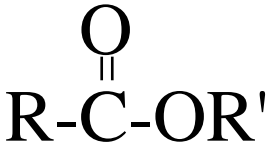
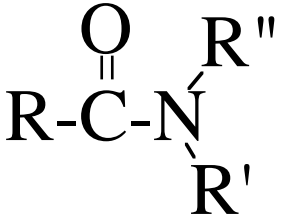
Amines	$R-NH_2$
Carboxylic Acids	

R′− or R− represents any generic carbon atom bonded in the functional group



Organic Molecules

Common Functional Groups

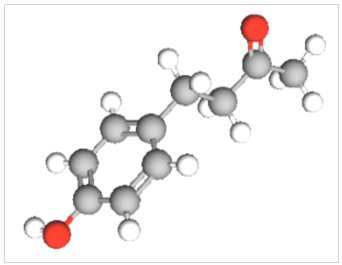
Name	General Formula
Aldehydes	
Ketones	
Carboxylic Acids	
Esters	
Amides	

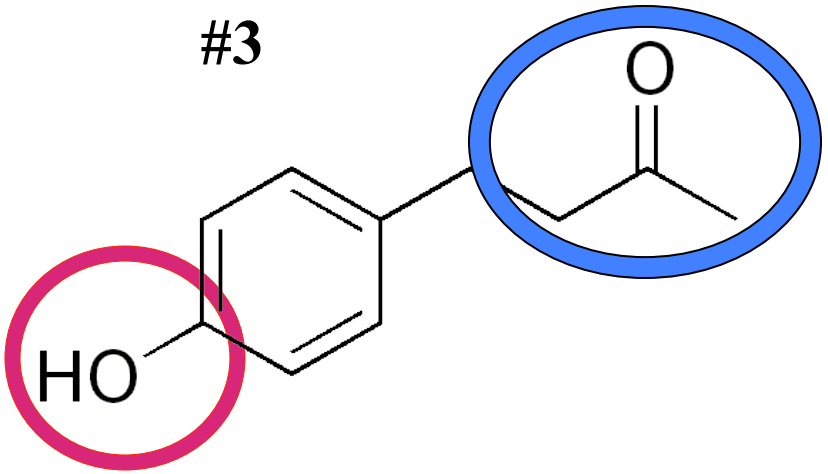
R′− or R− represents any generic carbon atom bonded in the functional group

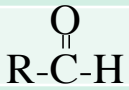
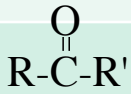
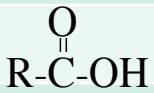
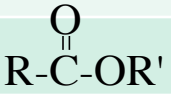
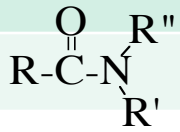
QUESTION

#3

Select the function(s) in the molecule





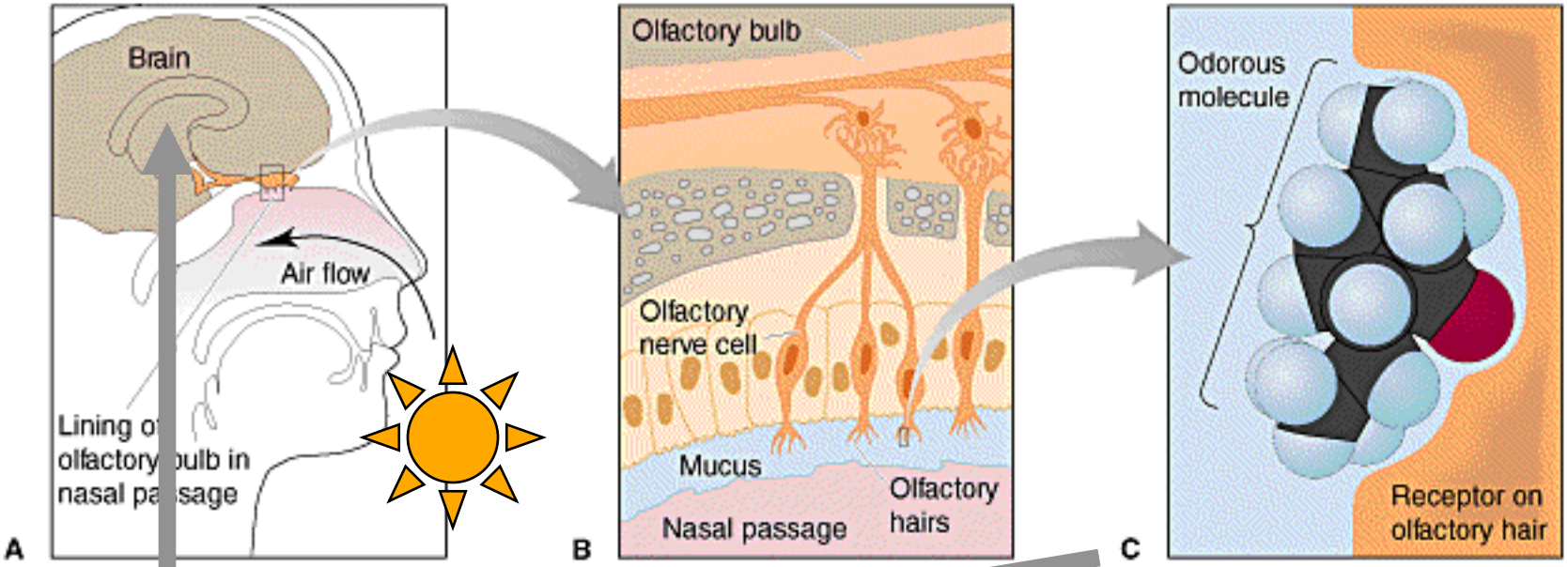
	Alcohol	R−OH
	Ether	R−O−R′
	Amine	$R-NH_2$
	Aldehyde	
	Ketone	
	Carboxylic Acid	
	Ester	
	Amide	

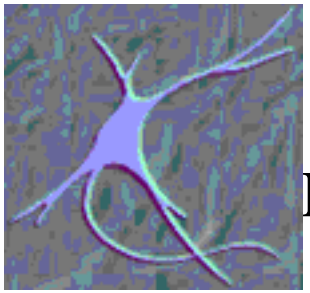
http://chemconnections.org/general/chem108/o-chem%20tutorial/Screen%20Shot%202018-12-07%20at%203.54.07%20PM.png

Detecting stuff we cannot see: the Sense of Smell

Models, Theories & Interactions

http://chemconnections.org/organic/chem226/Labs/Smell/smell-links.html

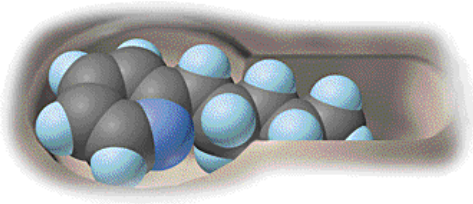




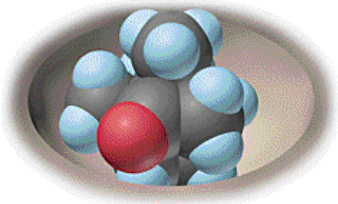
Structure-Odor Relationships

Karen J. Rossiter, Chem. Rev., 1996, 96, 3201-3240

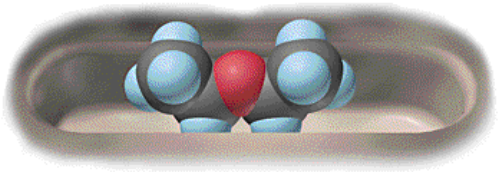
Historical view of a few smell receptors.



Floral



Camphor-like



Ethereal

4 October 2004

The Nobel Assembly at Karolinska Institutet has today decided to award

The Nobel Prize in Physiology or Medicine for 2004

jointly to

Richard Axel and Linda B. Buck

for their discoveries of

"odorant receptors and the organization of the olfactory system"

http://chemconnections.org/organic/chem226/Labs/Smell/ChemComm.html

Organic Functions & Smell Receptors.

Organic Chemistry

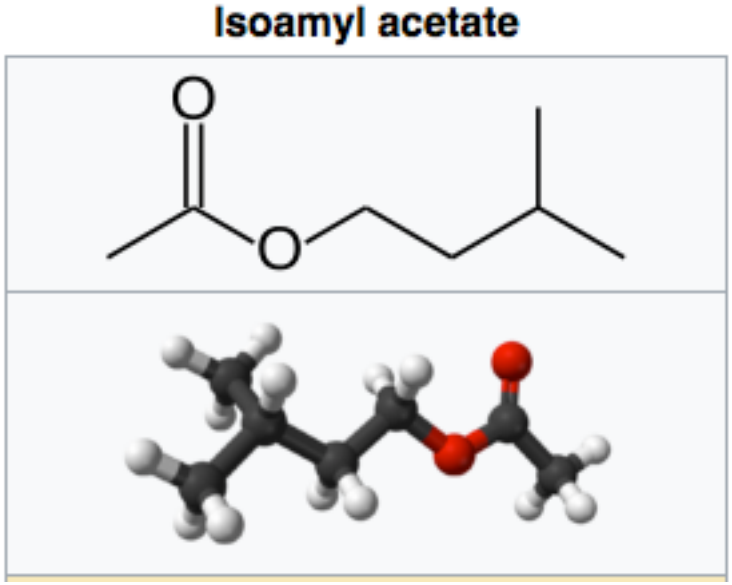
Table of organic compounds and their smells

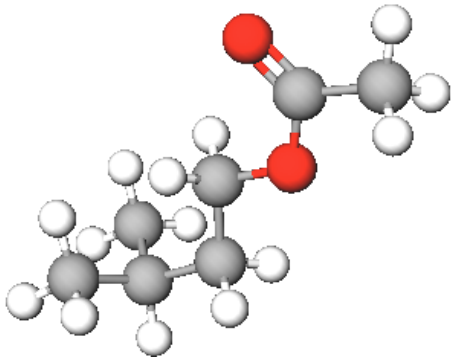
	ALKANES		ALKENES	ALCOHOLS		ALDEHYDES				KETONES		CARBOXYLIC ACIDS		HALOALKANES			THIOLS	AMINES		NITRILES	LACTONES
	-ane	cyclo -ane	-ene	-anol	-an-2-ol	-anal	2-methyl -anal	3-(4-t-butylphenyl) -anal	-enal	-an-2-one	methyl -an-2-one	-anoic acid	-enoic acid	chloro -ane	bromo -ane	iodo -ane	-anethiol	-anamine	diamino -ane	-anenitrile	-anolide
meth- 1 carbon	none	doesn't exist	carbene is too unstable to smell	ABSOLUT VODKA	doesn't exist	DANGER FORMALDEHYDE	doesn't exist	doesn't exist	doesn't exist	doesn't exist	doesn't exist	PUNGENT & PENETRATING	doesn't exist	TOXIC & MILDLY SWEET	LIKE CHLOROFORM	SWEET, ACRID			?		doesn't exist
eth- 2 carbons	none	doesn't exist		ABSOLUT VODKA	doesn't exist	FRUITY, ETHEREAL	doesn't exist	doesn't exist	doesn't exist	doesn't exist	doesn't exist	VINEGAR	doesn't exist	MILDLY SWEET	SWEET, ACRID	ETHEREAL	SKUNK			ETHEREAL	doesn't exist
prop- 3 carbons	none			ABSOLUT VODKA	RUBBING ALCOHOL	IRRITATING GREEN COFFEE	WET CEREAL	ATTRACTS SPERM	BURNED GREASE	NAIL VARNISH REMOVER	doesn't exist	SLIGHTLY RANCID	SHARP	MILDLY SWEET	SWEET	SHARP, UNIQUE				ETHEREAL	none
but- 4 carbons	none				WINE	PUNGENT BANANA		LILY	PUNGENT & SUFFOCATING	BUTTERSCOTCH	LIKE NAIL VARNISH REMOVER	RANCID BUTTER	BROWN SUGAR	SHARP	PLEASANT, SWEET	SHARP, UNIQUE			DEAD ANIMALS	SUFFOCATING	
pent- 5 carbons	STARTING FLUID	PLEASANT		STRONG SWEET	(S)- and (R)- enantiomers	PUNGENT NUTS & CHOCOLATE	FRESHLY CUT GRASS	?		&	MINT (4-methyl-)	DISGUSTING		MILD	PLEASANT, SWEET		ROASTED GARLIC		DEAD ANIMALS & URINE		HERBAL
hex- 6 carbons	STARTING FLUID	SWEET		FRESHLY CUT GRASS		FRESHLY CUT GRASS	FRESHLY CUT GRASS	?		ATTRACTS MICE	(3-methyl-)	GOATS	ARMPITS (WHEN 3-METHYLATED)	AROMATIC	SLIGHTLY SWEET	?	BURNED		ROTTING FISH		&
benzene different naming system is used	n/a	n/a	Benzene	SICKENINGLY SWEET AND TARRY Phenol	doesn't exist			?	doesn't exist	doesn't exist	Acetophenone	BALSAMIC	doesn't exist		AROMATIC			Aniline	TOXIC, AROMATIC	Benzonitrile	doesn't exist
hept- 7 carbons				FRESHLY CUT GRASS	(S)- and (R)- enantiomers	STRONG, FRUITY COGNAC	(2,6-dimethyl-heptanal)	?	ALMOND BUTTER	&	BAD (6-methyl-)	RANCID	ARMPITS (WHEN 3-METHYLATED)	none	SLIGHTLY SWEET	none					CARAMEL &
oct- 8 carbons	PETROL			PENETRATING, SWEET	(S)- and (R)- enantiomers	STRONG, CITRUS-LIKE	?	?		-2-one petrol -3-one herb butter	?	&	ARMPITS	none		SEAWEED	STENCH				
non- 9 carbons	DIESEL			CITRUS		ATTRACTS MOSQUITOES		?	OLD PEOPLE	MILK	?	RANCID	ARMPITS	none	none	none	OBNOXIOUS				
dec- 10 carbons	JET FUEL			CITRUS FLOWERS	?	BUCKWHEAT		?	ATORA TALLOW	?	?		ARMPITS	none	none	none	OBNOXIOUS				
undec- 11 carbons	NEW JET FUEL ALSO ANT 'PANIC' PHEROMONE	?		CITRUS FLOWERS	?	MAKES SPERM UNABLE TO FIND THE EGG	KUMQUATS	?	&	ALGERIAN OIL OF RUE	?	WAXY	PUNGENT & PENETRATING	UNIQUE & UNPLEASANT	none	MOUSE PHEROMONE	OBNOXIOUS				&
dodec- 12 carbons		MUSTY		FLOWERS	?		?	?	&	?	?	BAY OIL	FATTY	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS				&
tridec- 13 carbons	STINK BUG PHEROMONE	UNIQUE; FOUND IN ROSES		PLEASANT	?	GRAPEFRUIT PEEL	ROASTED	?	?	WAXY	?		?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none		ANGELICA ROOT
tetradec- 14 carbons	KAPOK BUSH FLOWERS	none			?		?	?	?	?	?	WAX & NUTMEG	?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none		CEDAR WOOD
pentadec- 15 carbons	TAMARIND (ANT-CALMING PHEROMONE)	?		ABSOLUT VODKA	?	FRESH	?	?	CORIANDER	CELERY	?	BIOMARKER FOR DAIRY CONSUMPTION (No smell)	?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none		MUSK

Version 1.2 Produced by James at jameskennedymonash.wordpress.com. Visit website for more infographics. Free to use!

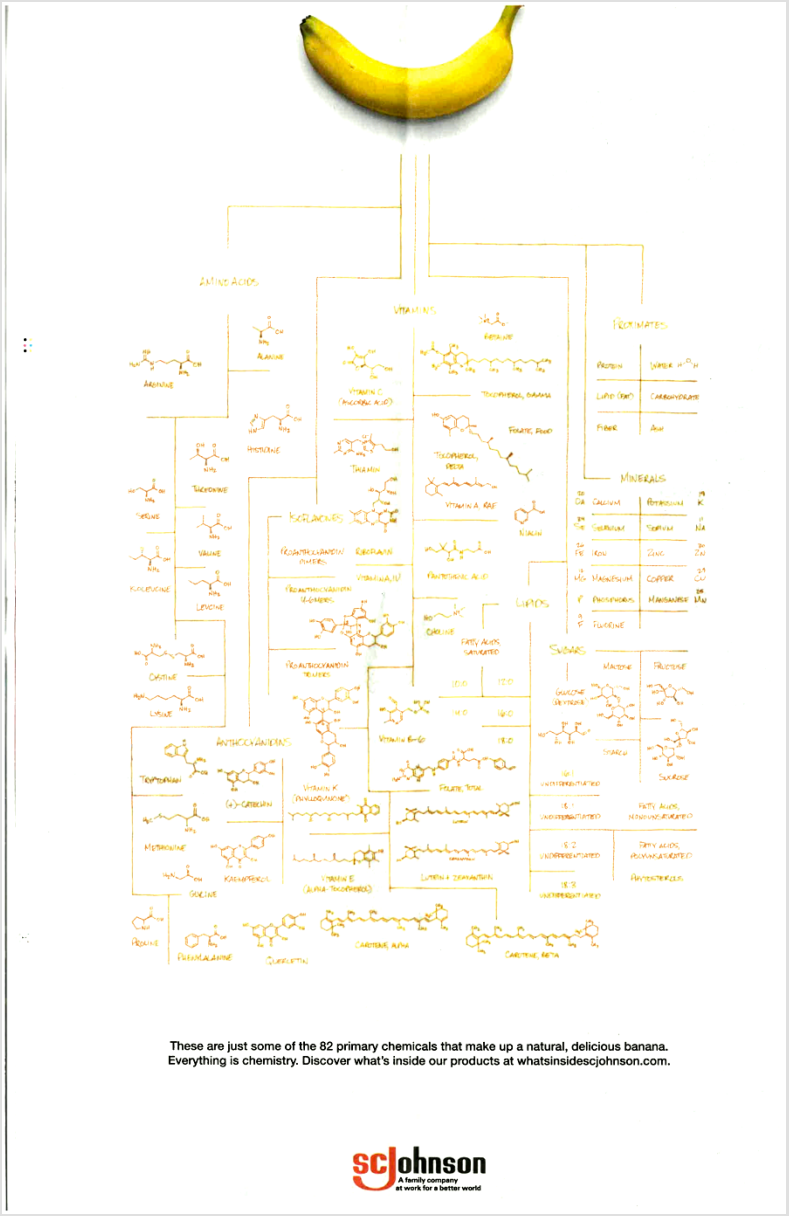
One molecule, one function: One Smell Receptor

Isoamyl acetate, also known as isopentyl acetate, is formed from isoamyl alcohol and acetic acid. It is a colorless liquid that is only slightly soluble in water, but very soluble in most organic solvents. Isoamyl acetate has a strong odor which is also described as similar to both banana and pear.[3] Banana oil may be either pure isoamyl acetate, or flavorings that are mixtures of isoamyl acetate, amyl acetate, and other flavors.

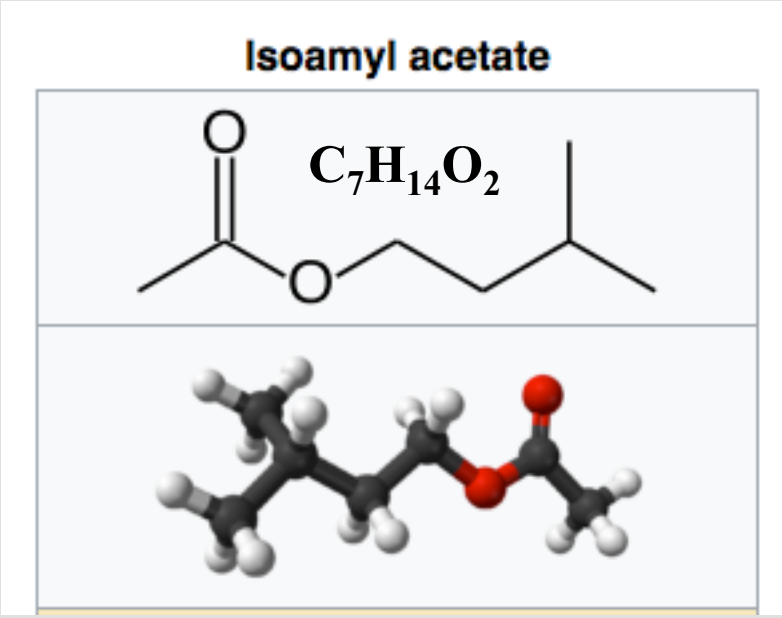




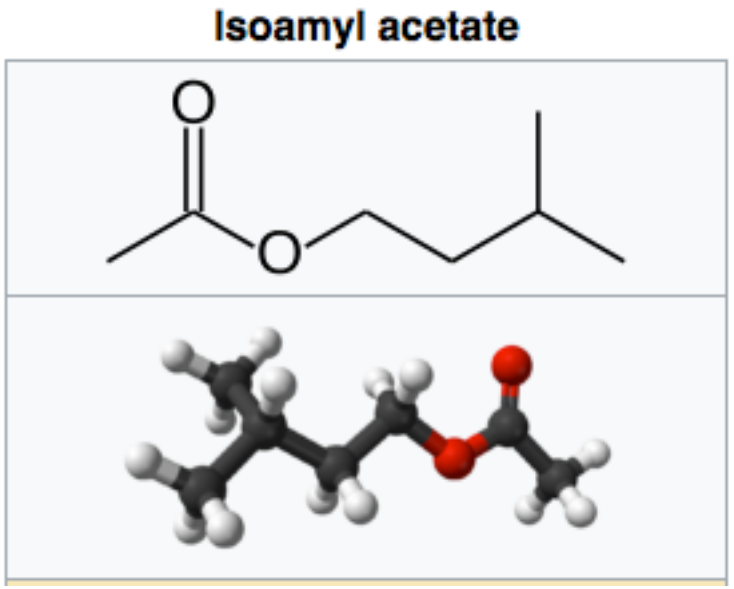
$C_7H_{14}O_2$

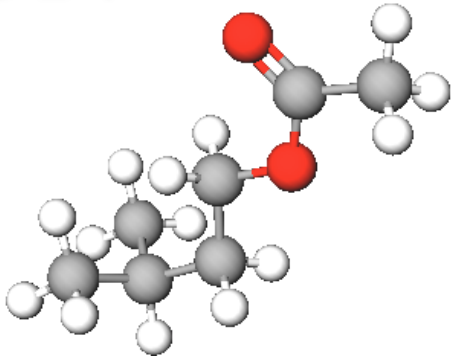


One molecule among 82 primary chemicals found in bananas:



QUESTION #4





$C_7H_{14}O_2$

The function in isoamyl acetate's structure is a(n):

A.Alcohol

B.Aldehyde

C.Ketone

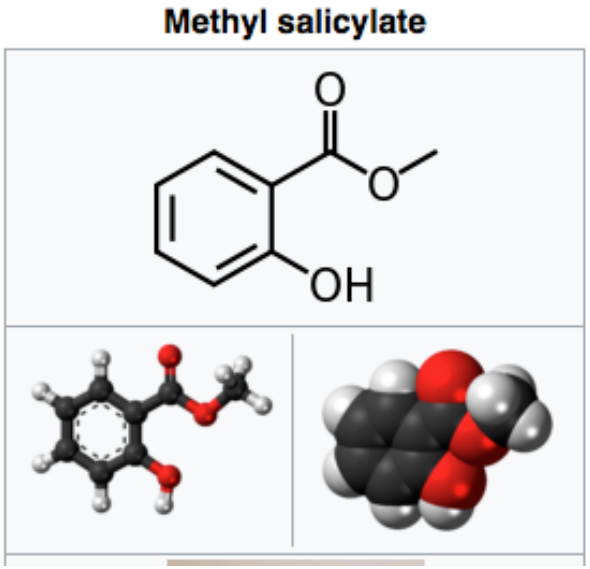
D.Ester

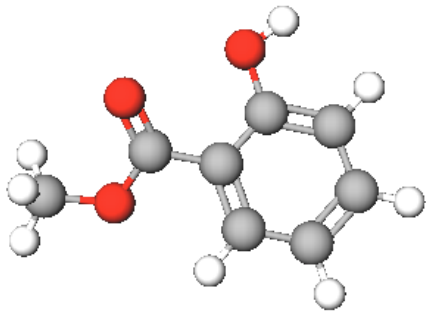
E.Carboxylic Acid

http://chemconnections.org/general/chem108/o-chem%20tutorial/Screen%20Shot%202018-12-07%20at%203.54.35%20PM.png

One molecule, two functions: One Smell Receptor

Methyl salicylate (oil of wintergreen or wintergreen oil) is naturally produced by many species of plants, particularly wintergreens. It is also synthetically produced, used as a fragrance, in foods and beverages, and in liniments.

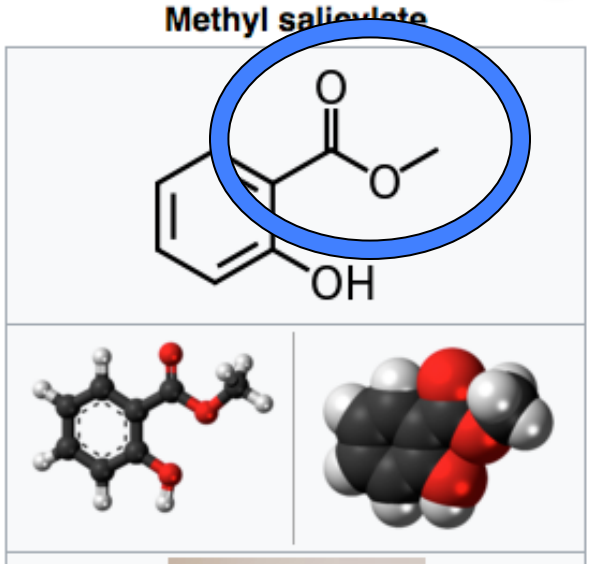


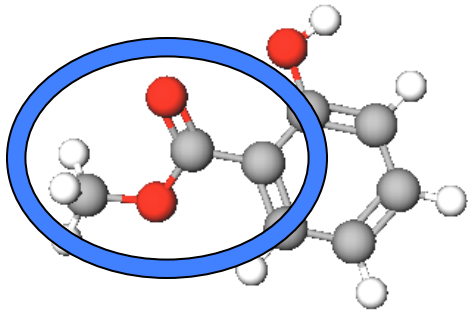


$C_8H_8O_3$

QUESTION

#5





$C_8H_8O_3$

One of the functions, an ester, is circled. What is the other function?:

A.Alcohol

B.Ether

C.Ketone

D.Aldehyde

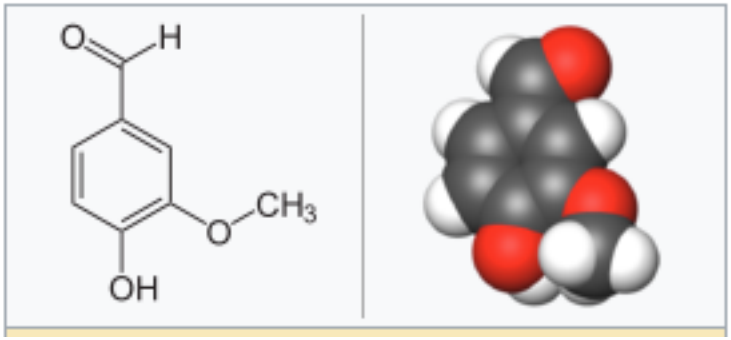
E.Carboxylic Acid

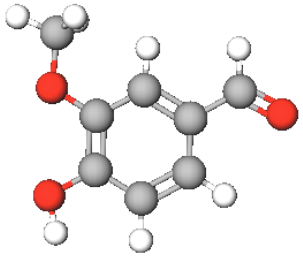
http://chemconnections.org/general/chem108/o-chem%20tutorial/Screen%20Shot%202018-12-07%20at%203.54.53%20PM.png

One molecule, three functions: One Smell Receptor

An extract of the cured, full-grown, unripe fruit of an orchid produces a popular flavoring. The natural extract sells for ~ $1500/kg versus ~ $20/kg for the synthetic version. The structure of the compound that is responsible for the smell/flavor is shown to the right. The Guinness Book of World Records once listed this compound as having the lowest smell detection limit of all chemicals (2 x 10^{-11} g per 1,000 cm^3 of air).

Vanillin



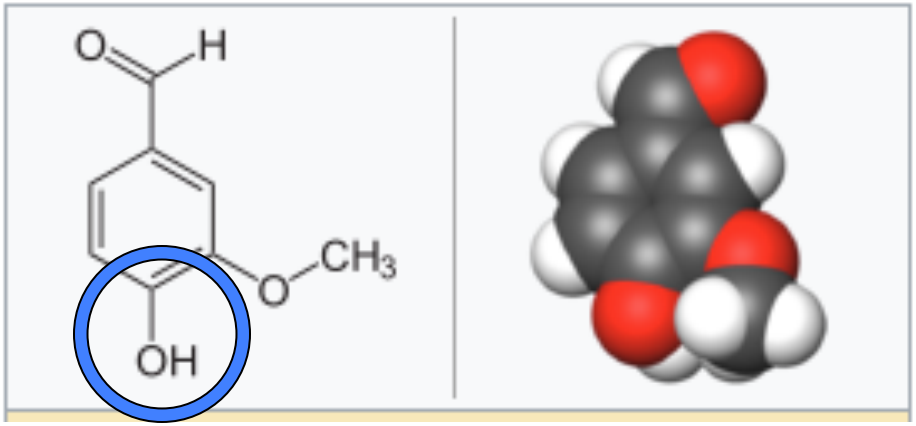


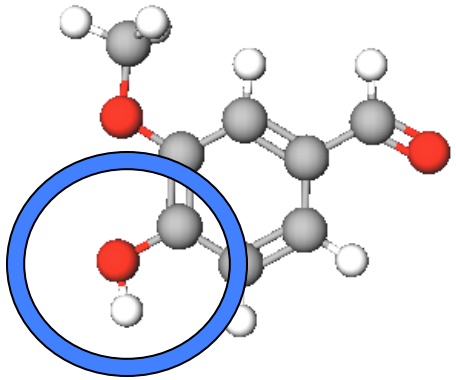
Bonus:
The space (volume) of the Oakland Coliseum Arena, aka Oracle Arena, is approximately 90,000,000 ft^3. If 1.00g of the compound were released at center court, and was completely and evenly dispersed throughout the building, would you smell it sitting in sec. 204, row H, seat 121? Show your calculation. (1 ft^3 = 0.0283 m^3)

QUESTION

#6

Vanillin



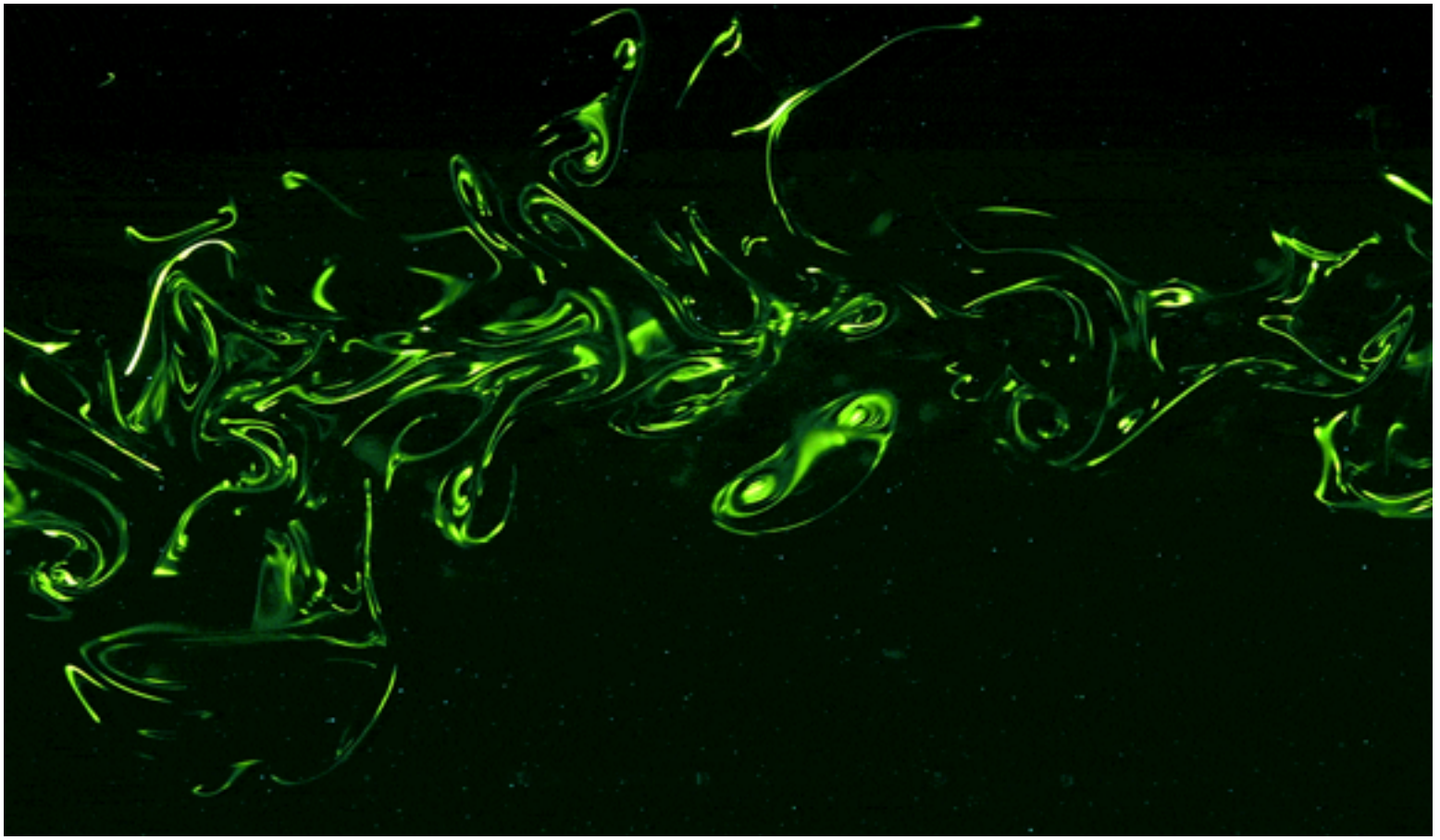


One of the functions, an alcohol, is circled.
What are the other two functions?:

A.Aldehyde + Ketone
B.Carboxylic Acid + Ester
C.Ketone + Ether
D.Aldehyde + Ether
E.Carboxylic Acid + Aldehyde

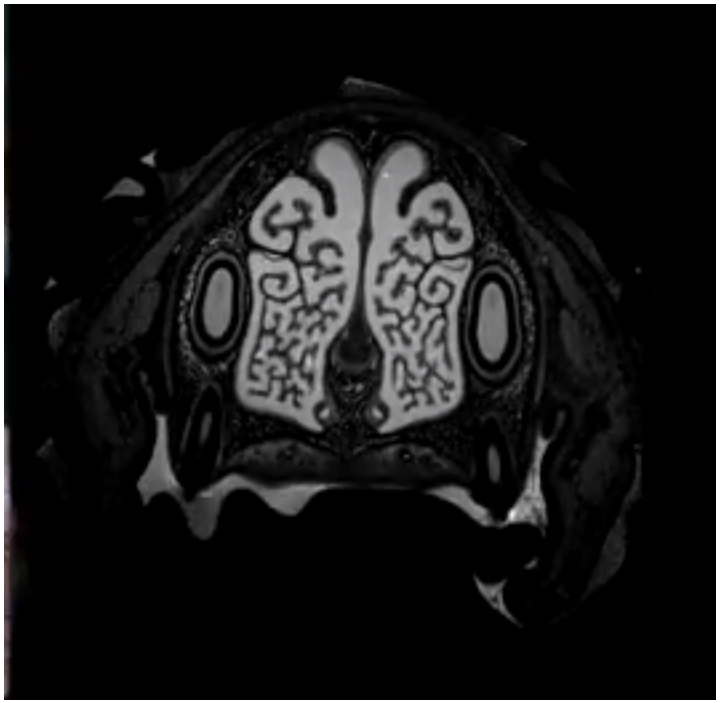
http://chemconnections.org/general/chem108/o-chem%20tutorial/Screen%20Shot%202018-12-07%20at%203.55.14%20PM.png

What a smell looks like



https://www.youtube.com/watch?v=58U52lDTuvk&list=PLgawtcOBBjr9I-NDoUX-HmTQr_VN465G2&index=3

Inside the extraordinary nose of a search-and-rescue dog



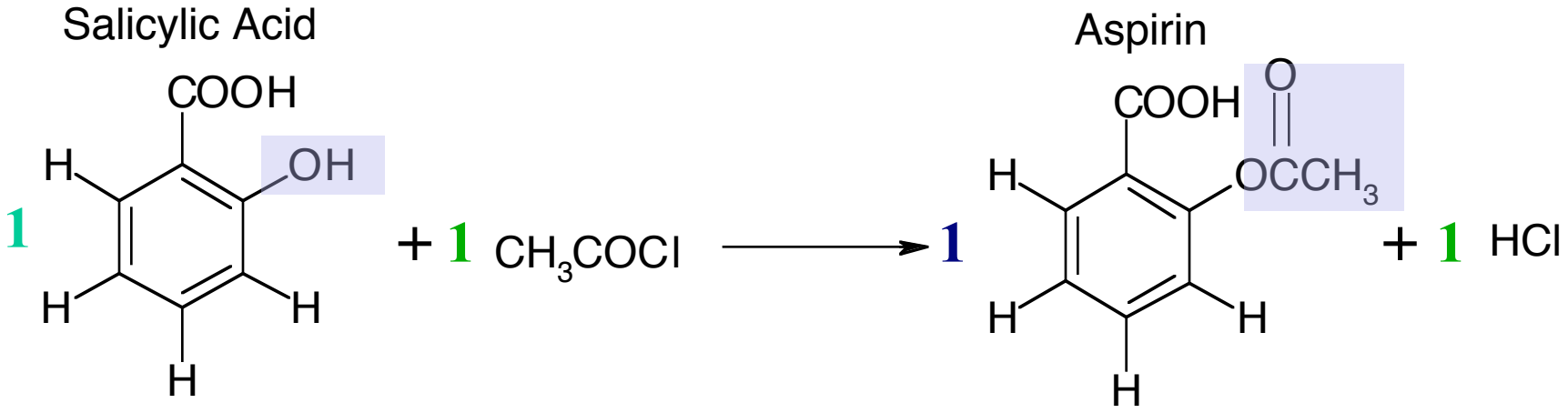
https://www.youtube.com/watch?v=FLH36ML8IEU

Dogs Can Smell Cancer - Secret Life of Dogs - BBC

https://www.youtube.com/watch?v=e0UK6kkS0_M

Mass Calculations: Reactants ⟷ Products

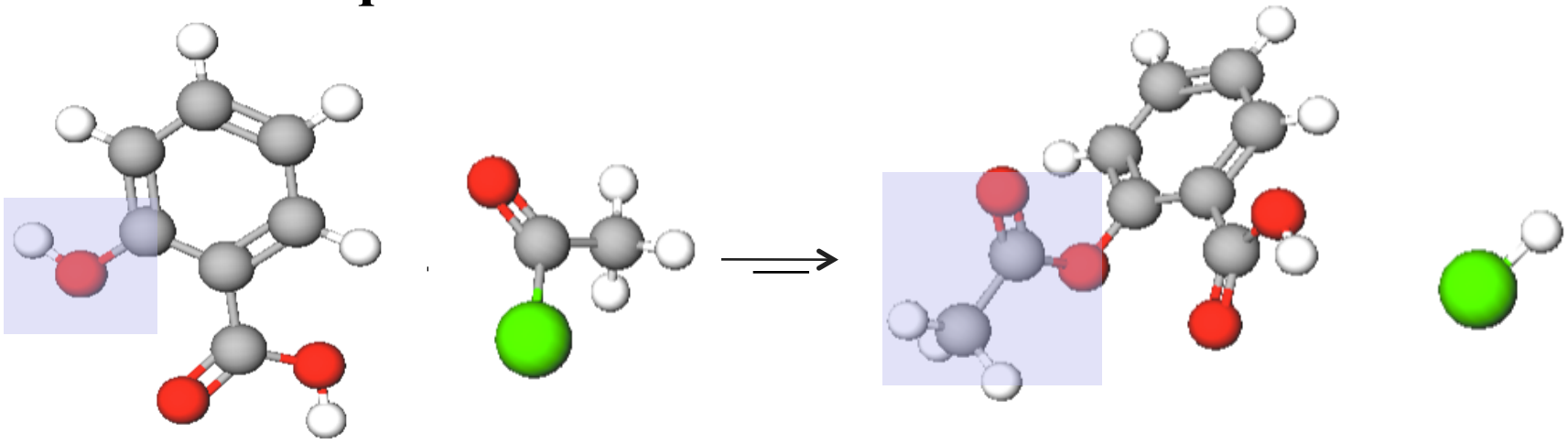
- **How many grams of aspirin are theoretically produced from 6.0 g of salicylic acid with an excess of acetyl chloride, C_2H_3OCl?**
- **Balanced Equation:**



$C_7H_6O_3$	C_2H_3OCl	$C_9H_8O_4$	HCl
MW = 138.12	MW = 78.49	MW = 180.15	MW= 36.45

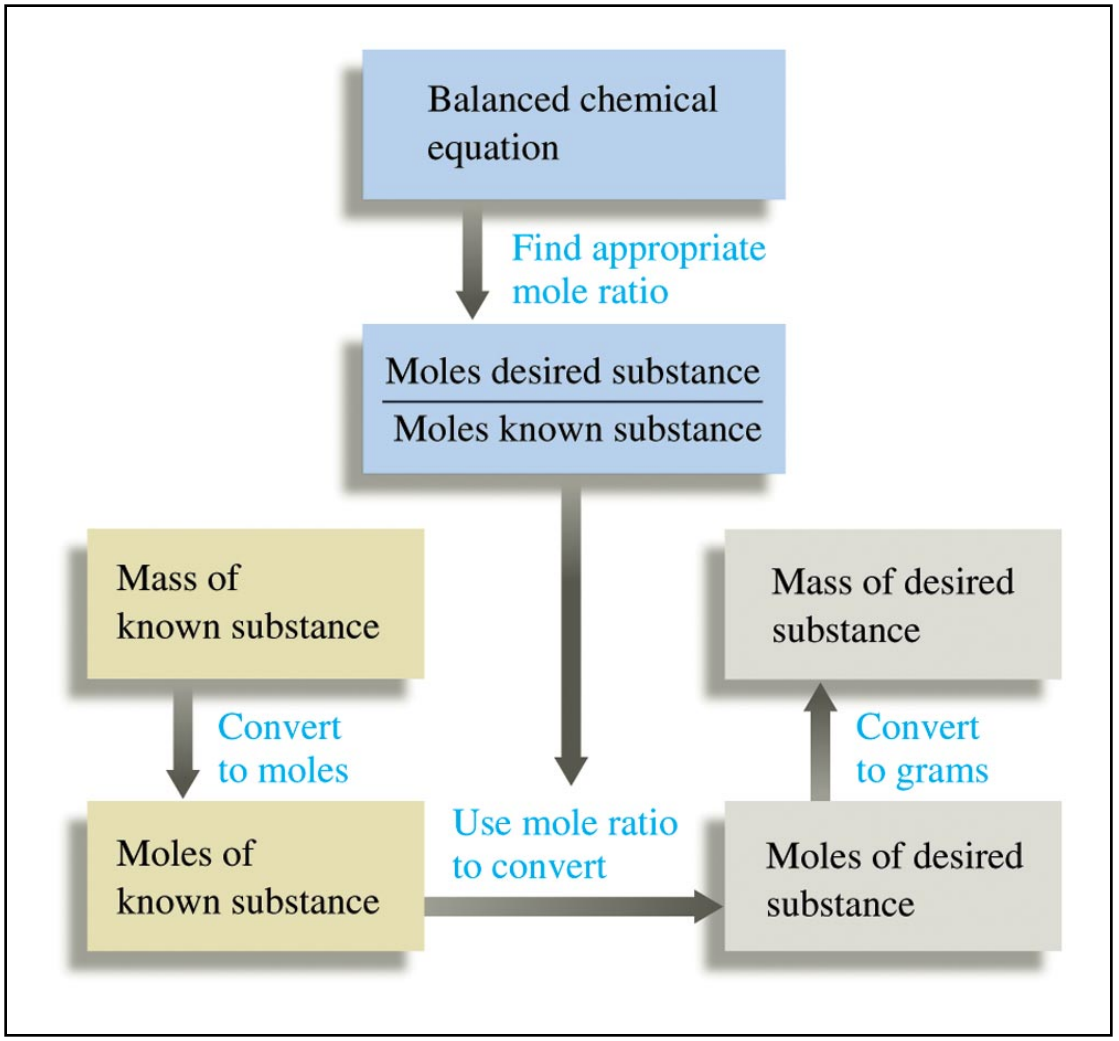
Mass Calculations: Reactant ⟶ Product

- **How many grams of aspirin are theoretically produced from 6.0 g of salicylic acid with an excess of acetyl chloride, C_2H_3OCl?**
- **Balanced Equation:**



$C_7H_6O_3$	C_2H_3OCl	$C_9H_8O_4$	HCl
MW = 138.12	MW = 78.49	MW = 180.15	MW= 36.45

Mass Calculations: Reactants ⟷ Products



Theoretical (Yield) Mass Calculations
Reactant → Product

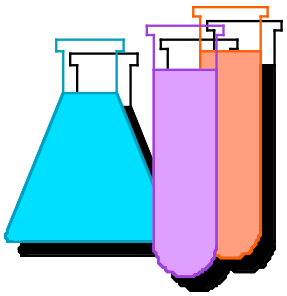
grams (Reactant) → grams (Product)

Moles

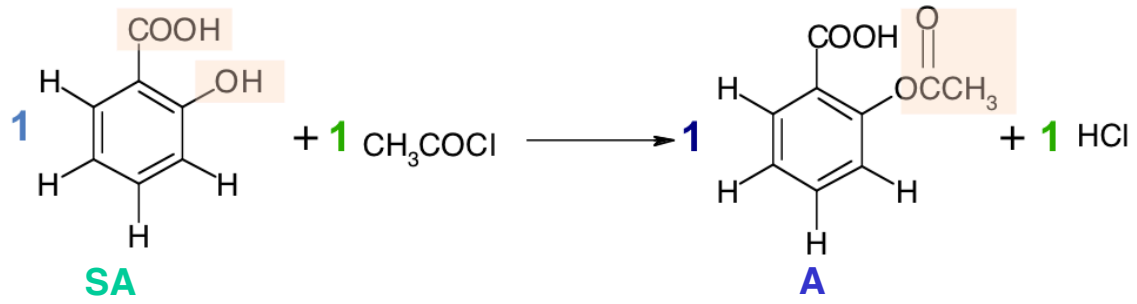
Molar Mass

Stoichiometry

grams (R)	1 mol (R)	? mol (P)	grams (P)	= ? grams (P)
	grams (R)	? mol (R)	1 mol (P)	
	(*Divide*) by Molar Mass (R)	*"Gatekeepers" from Balanced reaction*	(*Multiply*) by Molar Mass (P)	



Mass Calculations:



grams (Salicylic Acid) ⟶ grams (Aspirin)

Moles
Molar Mass
Stoichiometry

$C_9H_8O_4$
MW = 180.15

6.0 grams (SA) | **1 mol (SA)** | **1 mol A** / **1 mol SA** | **grams (A)** (Molecular Weight A) | **1 mol (A)** = **? (A)**

grams (SA) (Molecular Weight SA)

$C_7H_6O_3$

MW = 138.12

"Gatekeeper"

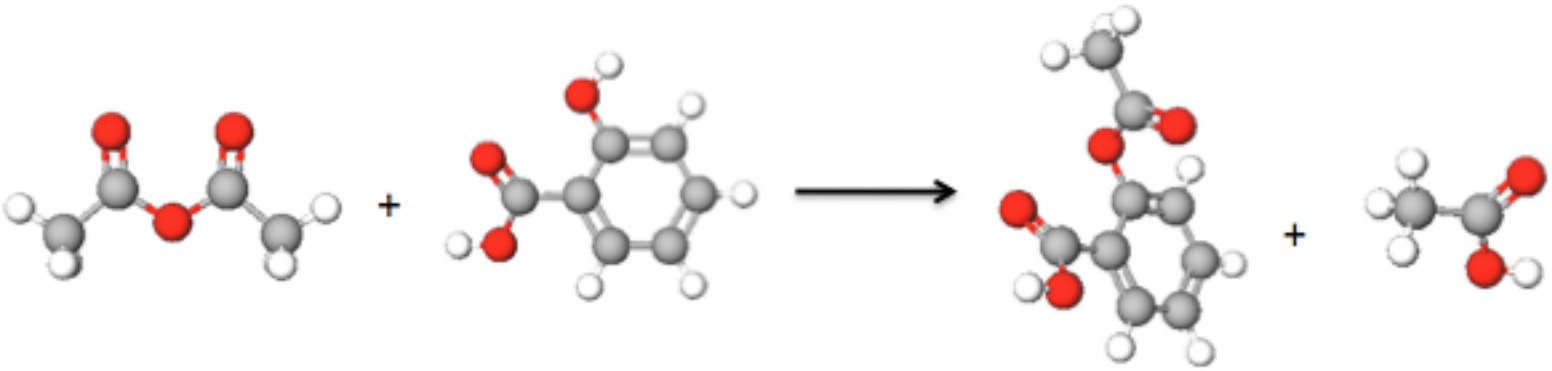
7.8 g aspirin

QUESTION

http://chemconnections.org/general/chem108/o-chem%20tutorial/Screen%20Shot%202018-12-07%20at%203.55.53%20PM.png

#7

- **How many grams of aspirin can be theoretically produced from 5.0 g of salicylic acid reacting with an excess of acetic anhydride, $C_4H_6O_3$?**
- **Balanced Equation:**



salicylic acid

aspirin

$C_4H_6O_3$	$C_7H_6O_3$	$C_9H_8O_4$	$C_2H_4O_2$
MW = 102.09	MW = 138.12	MW = 180.15	MW= 60.05

A) 3.8 g **B) 5.0 g** **C) 6.5 g** **D) 7.8 g**

Percent Yield

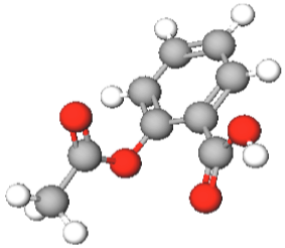
- **In synthesis as in any experiment, it is very difficult and at most times impossible to be perfect. Therefore the actual yield (g) is measured and compared to the theoretical calculated yield (g). This is the percent yield:**

- **% Yield = actual (g) / theoretical (g) x 100**

QUESTION

http://chemconnections.org/general/chem108/o-chem%20tutorial/Screen%20Shot%202018-12-07%20at%203.56.16%20PM.png

#8



- Kaitlyn's synthesis of aspirin, $C_9H_8O_3$, produced 5.90g. The calculated theoretical yield was 6.50g; what is her % yield?

A) 47.5% B) 80.3% C) 90.8% D) 110%