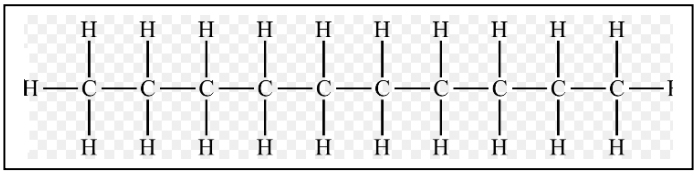
Naming organic compounds with functional groups and writing semi-structural formulae.
Lesson 1b

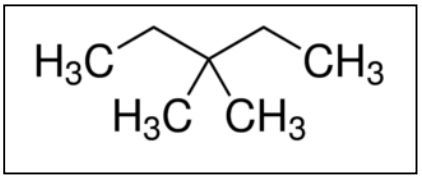
Semi-structural formulae represent an unambiguous way of writing the structure of an organic molecule in a simple short-hand way.



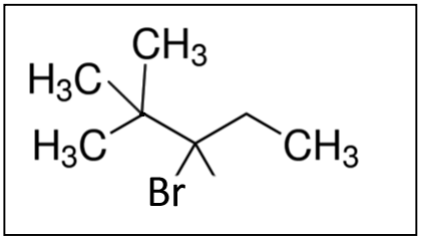
For example, consider the molecule of decane shown on the right.
The semi-structural formula shows the group of atoms and the order in which they are attached.

Decane can be written as $CH_3CH_2CH_2CH_2CH_2CH_3CH_2CH_2CH_2CH_3$ or more succinctly as $CH_3(CH_2)_8CH_3$

Brackets are used in two ways, they can reduce the amount of work in writing the formula, as in the example given, and to remove ambiguity from a structure. Brackets can also signify a group of atoms that come off the preceding carbon.
Take the example of 3,3-dimethyl pentane, shown on the right. It can be written as $CH_3CH_2C(CH_3)_2CH_2CH_3$

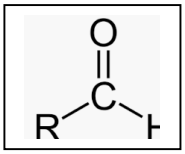


3-bromo-2,2,3-trimethylpentane can be written as $(CH_3)_3CCBr(CH_3)CH_2CH_3$ or the less condensed version of $CH_3C(CH_3)_2CBr(CH_3)$. Since there is no ambiguity and both formulae will lead to drawing the exact same molecule both are applicable.

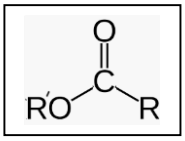


Some pints to note when writing condensed or semi-structural formulae.

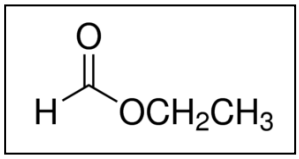
Aledhydes are written as CHO as opposed to COH which implies a hydroxyl group.



Esters are written as R′COOR and not as the appear R'OCOR
If it's a methanoate ester such as ethyl methanoate then it must be written so that it is unambiguous between an acid and an ester.



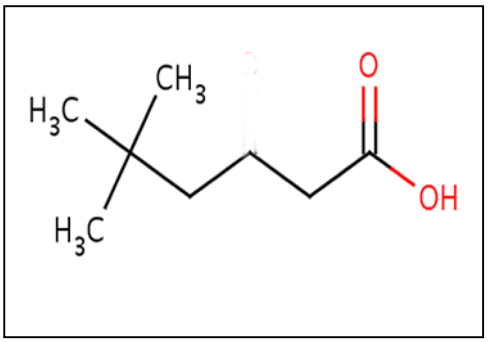
eg. Writing ethyl mathanoate in condensed form it is easy to confuse it with porpanoic acid. CH_3CH_2COOH so write it so that the hydrogen appears first $HCOOCH_2CH_3$



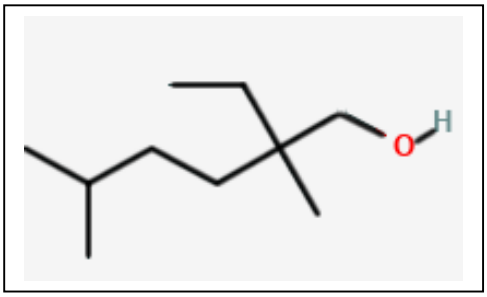
A carboxylic acid is shown as R'COOH. Eg. Propanoic acid CH_3CH_2COOH

Alcohols have an OH. Eg. Propan-2-ol is written as $CH_3CH(OH)CH_3$ or propan-1-ol is $CH_3CH_2CH_2OH$
A ketone is written as R'COR
An ether is shown as R'OR

1) Name the following and write the condensed or semi-structural formula for each of the molecules shown.

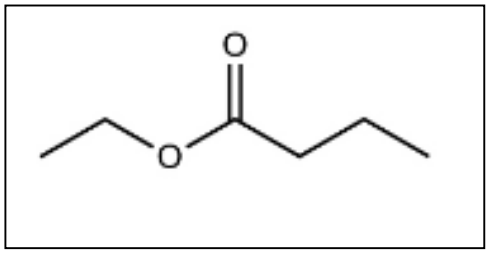


5,5-dimethylhexanoic acid
$(CH_3)_3C(CH_2)_3$ COOH or $CH_3C(CH_3)_2CH_2CH_2CH_2COOH$

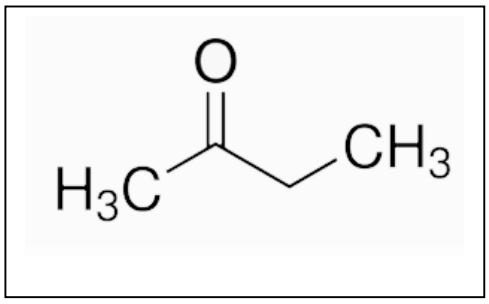


2-ethyl-2,5-dimethylhexan-1-ol
$CH(CH_3)_2CH_2CH_2C(CH_2CH_3)(CH_3)CH_2OH$

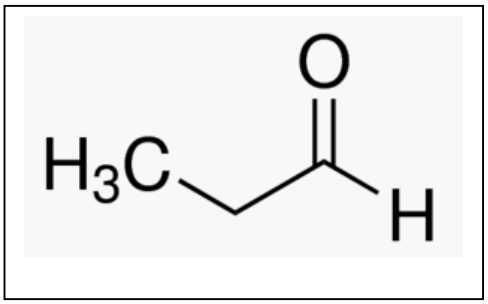
2) Write the condensed formulae of the following molecules



$CH_3CH_2CH_2COOCH_2CH_3$

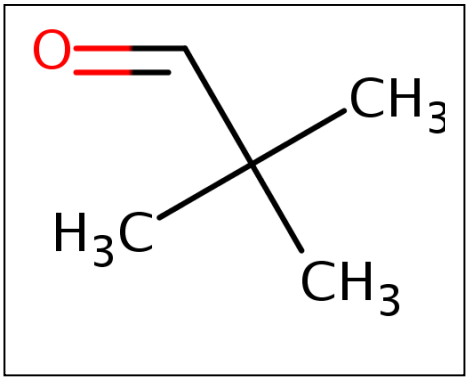


$CH_3COCH_2CH_3$

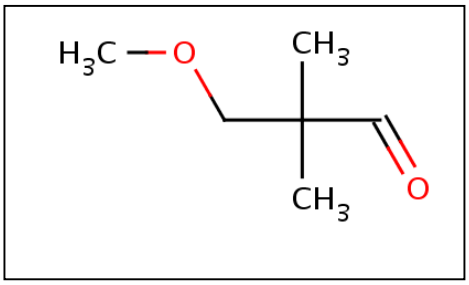


CH_3CH_2CHO (the CHO implies an aldehyde)

$CH_3C(CH_3)_2CHO$ (CHO indicates an aldhyde)



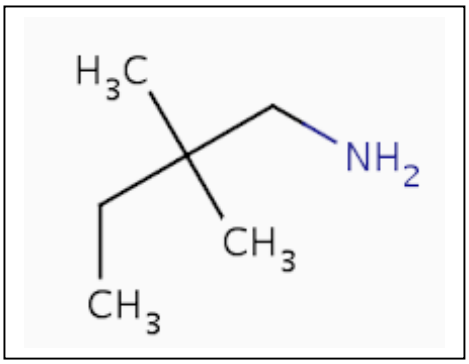
$CH_3OCH_2C(CH_3)_2CHO$



3) Complete the following

a)

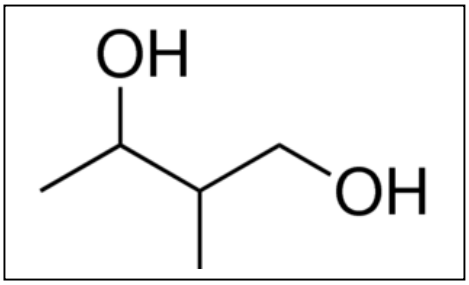
Name 2,2-methylbutan-1-amine



Condensed formula
$CH_3CH_2C(CH_3)_2CH_2NH_2$
Brackets (around the NH_2) are not necessary as it is not ambiguous , the terminal NH_2 must be attached

b)

Name *2-methylbutan-1,3-diol*



Condensed formula
$CH_3CH(OH)CH(CH_3)CH_2OH$
Brackets (around the OH) are not necessary as it is not ambiguous , the terminal OH must be attached to the end CH_2

c) Name the compound with the condensed formula $(CH_3CH_2)_2CH(CH_2)_4CH_2OH$

6-ethyloctan-1-ol