Exercise sheet 1: From atoms to molecules

Organic chemistry for bioinformatics, lecture 1. Exercises marked *(bonus)* are optional.

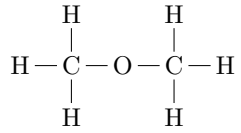
Exercise 1: Valence electrons and bonds

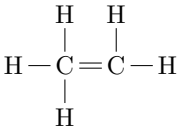
Use a periodic table. For each element give a) its name, b) the number of valence electrons, c) the number of electrons missing for a full outer shell, d) the number of covalent bonds it usually forms in organic molecules, and e) the number of lone pairs it then keeps.

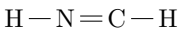
	a) name	b) valence e^-	c) missing e^-	d) bonds	e) lone pairs
Cl					
C					
H					
N					
O					
S					
P					

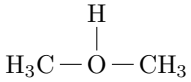
Exercise 2: Valency check

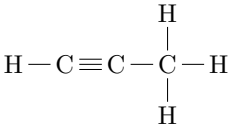
Which of the structures a)–i) are *not* possible as drawn (neutral molecules, no charges)? Mark the atom(s) with a wrong number of bonds and say what is wrong.
Tip: count bonds, not lines. A double bond counts twice, and wedges and dashes are bonds too.

a) 

b) 

c) 

d) 

e) 

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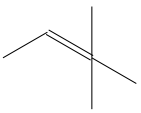
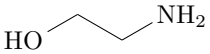
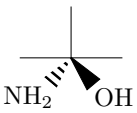
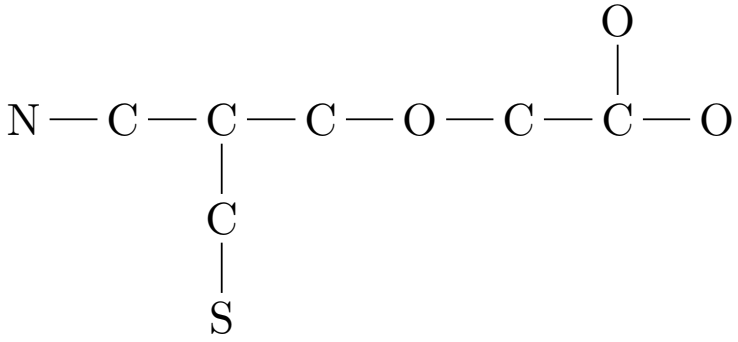
g) 

h) 

i) 

Exercise 3: Fill in the missing bonds

The drawing shows how the heavy atoms (C, N, O, S) of a molecule are connected. All connections are drawn as single lines and all hydrogens are left out. The molecular formula is $C_xH_9N_yO_zS$.



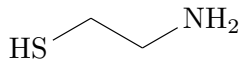
a) Determine x, y and z.

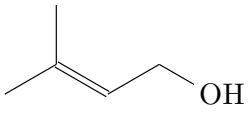
b) How many double bonds must the molecule contain (a triple bond counts as two)?
Hint: every ring or double bond "costs" two H. A saturated, open-chain molecule with n carbons has $2n + 2$ hydrogens; each N adds one more H, while O and S add none.

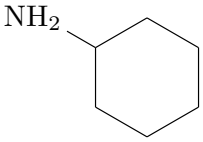
c) Complete the structure: add the multiple bonds and all hydrogens so that every atom has the right number of bonds. There is more than one solution.

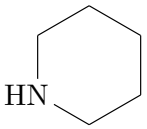
Exercise 4: Notations

For each molecule a)–d), write the molecular formula and draw the full Lewis (structural) formula with all atoms and all bonds.

a) 

b) 

c) 

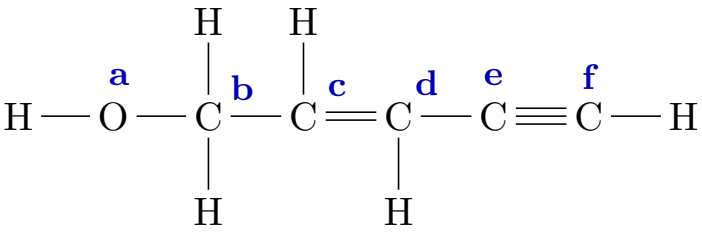
d) 

Exercise 5: Isomers of $C_4H_{10}O$

a) Draw all constitutional isomers of $C_4H_{10}O$ as skeletal formulas. How many are there? *Hint: first use the "two H" rule to check whether rings or double bonds are possible.*

b) *(bonus)* Which of your molecules contains a chiral carbon?

Exercise 6: Geometry



a) What is the geometry around each labelled atom a–f (tetrahedral, planar, linear or bent)? *Hint: count the neighbours (bonded atoms) and the lone pairs of each atom. A double or triple bond counts as one neighbour.*

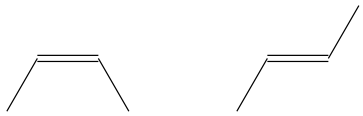
b) Which atoms together form the largest planar substructure, i.e. atoms that always lie in one plane, whatever the rotation around the single bonds?

c) Can this molecule exist as a cis and a trans isomer? Explain.

Exercise 7: Same or different?

For each pair a)–g): are the two drawings *constitutional isomers*, *stereoisomers* (cis/trans isomers or enantiomers) or *the same molecule*? Give a reason.

a)



b)



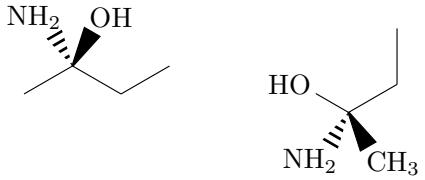
c)



d)



e)



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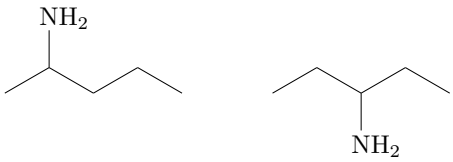

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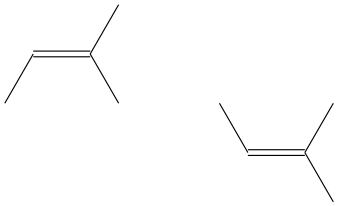

Exercise 8: Find the stereocentres

The molecules a)–e) are the steps of the adrenaline pathway (lecture 3); the 3D information is not shown. For each molecule give the molecular formula and mark every stereocentre (carbon with four different substituents).

