Organic Chemistry

Exercise 1

1. What are the electronic configurations of carbon, silicon, and chlorine in the ground state?

2. Draw a schematic energy level diagram of carbon in the ground state, along with an illustration of the orbitals that hold the valence electrons!

3. Schematically formulate the formation of sp, sp^2, and sp^3 hybrid orbitals! What are the resulting coordination geometries, according to the VSEPR model?

4. Schematically draw bonding models for methane, ethane, ethene, and ethyne, based on the valence bond model!

5. What is the difference between the carbon-carbon σ-bond and the π-bond in ethene?

6. Transfer: Draw a schematic and simplified MO energy level diagram of hydrogen (H_2)! Name the resulting molecular orbitals and schematically illustrate them according to the LCAO approach! What is the "bond energy", i.e., the total energy that stabilizes the covalent bond?

7. Draw a schematic MO energy level diagram of the hypothetical helium molecule (He_2) and compare it to the MO energy level diagram of hydrogen (H_2).

8. What are the two requirements that need to be respected when one derives molecular orbitals from linear combinations of atomic orbitals?

Reading Suggestions:

Clayden, Greeves, Warren, Wothers, *Oxford University Press*, **2001**, pp. 81–110.

Chimie Organique, Paul Arnaud, *Dunod Editeur*, **2009**, pp. 73–88.

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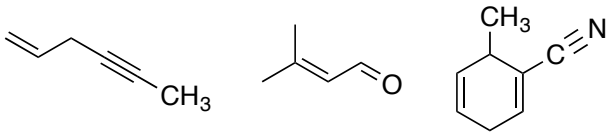
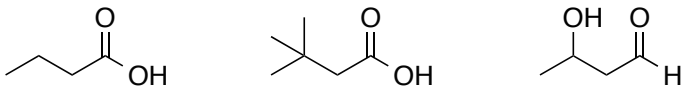
Exercise 2

1. What is the coordination geometry and hybridization of each carbon atom in the following molecules?



2. Give the molecular formulae of the following compounds:



3. Suggest detailed structures for the following molecules that indicate their three-dimensional shape: HCCH, CO_2, CH_2NCH_3, CHF_3, H_2O, CH_2CCH_2, $(CH_3)_3CBr$

4. Transfer: Can you explain – based on the molecular structure of H_2O – why water has a permanent dipole moment? Compared to other compounds with a similar molecular weight and structure (e.g. H_2S, M= 34,08 g/mol, Mp = -85.7°C, Bp = -60,2°C) water has got an exceptionally high melting and boiling point. Can you make give reasons based on the molecular structure of water? Please provide a sketch.

5. Draw schematic and simplified MO energy level diagrams of ethane and ethene, starting from two $H_3C\cdot$ fragments or two H_2C: fragments, respectively (just show the orbitals involved in the carbon-carbon bond(s), disregard all orbitals involved in C–H bonds)!

6. Transfer: Draw schematic and simplified MO energy level diagrams of bromomethane, starting from $H_3C\cdot$ fragments and an $Br\cdot$ atom, respectively (just show the orbitals involved in the carbon-carbon or carbon-bromine bonds)! Compare the diagram to the one of ethane, discuss and explain the differences.

Reading Suggestions:

Clayden, Greeves, Warren, Wothers, *Oxford University Press*, **2001**, pp. 81–110 & 151–179.

Chimie Organique, Paul Arnaud, *Dunod Editeur*, **2009**, pp. 73–103.

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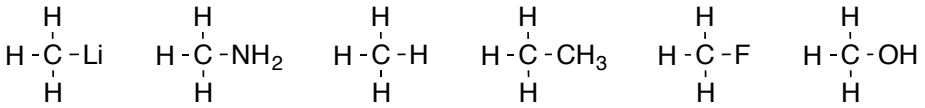
Exercise 3

1. Briefly describe the general electronegativity trends in the periodic table. A difference in electronegativity leads to a polarization of bonds and an uneven distribution of electron density. Sort the following chemical compounds in the order of increasing electron density on the carbon atom.

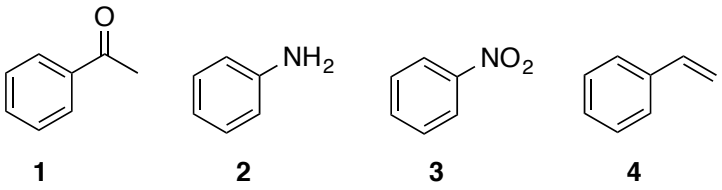


2. Draw the structure formulae for the following molecular formulae: $CH_2CHCH_2CHCHCH_3$ (1,4-hexadiene), CH_2CCH_2 (1,2-propadiene), and $CH_3CH_2CHCHCHCHCH_2CH_3$ (3,5-octadiene)! In the molecules you have drawn, highlight which double bonds are isolated, conjugated, or cumulated?

3. What are the differences between conjugated and isolated double bonds with respect to the electron density distribution, orbital overlap, and energy of the molecular orbitals? Explain on the basis of the following molecules: $CH_2CHCHCHCH_3$ (1,3-pentadiene) and $CH_2CHCH_2CHCH_2$ (1,4-pentadiene).

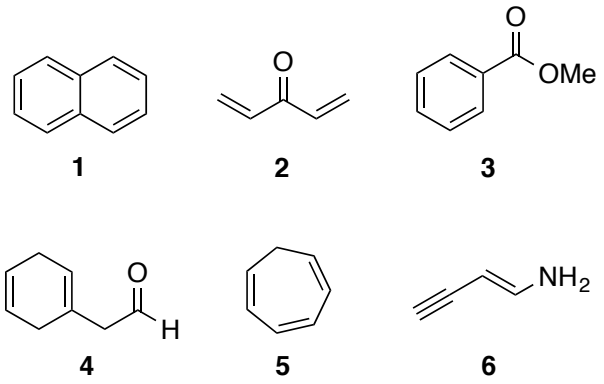
4. Draw schematic and simplified MO energy level diagrams of 1,3-butadiene and benzene. Draw representations that indicate how the p-orbitals overlap to form the molecular orbitals at the different energy levels of the MO diagram. How many nodes do you have at each level?

5. Draw all relevant resonance structures for the following compounds: acetophenone **1**, aminobenzene **2**, nitrobenzene **3**, and styrene **4**. Locate charges in these molecules and indicate with partial charges how the charge distribution looks? Indicate which structures are major and minor in contribution to the overall structure.



1 **2** **3** **4**

6. Transfer: Draw all relevant resonance structures for the following compounds **1–8**. Estimate the bond order for each bond form the resonance structures and indicate which compounds are aromatic.



1 **2** **3**

4 **5** **6**

Reading Suggestions:

Clayden, Greeves, Warren, Wothers, *Oxford University Press*, **2001**, pp. 81–110 & 151–179.

Chimie Organique, Paul Arnaud, *Dunod Editeur*, **2009**, pp. 73–103.