Self-assessment test for basic chemistry knowledge (solutions)

Part 1 – Analytical Chemistry

1. For the preparation of pretzels, a sodium hydroxide solution (mass share $\omega_{NaOH} = 4.0\ \%$) with a density $\rho(20\ °C)$ of 1.04 g/cm^3 is used. Calculate the concentration of this solution in mol/L (M(NaOH) = 40 g/mol).

   Assume a volume of 1 L. A sodium hydroxide solution then weights: $m = \rho \cdot V = 1.04\,\frac{g}{cm^3} \cdot 1000\ dm^3 = 1040g.$

   Notice that this is the mass of the whole solution. NaOH is just 4.0 % of that, which is 41.6 g pure NaOH in that solution.

   Convert this into molar quantities: $n = \frac{m}{M} = \frac{41.6\ g}{40\ g/mol} = 1.04\ mol.$ Because our assumption was a volume of 1 L, the molar concentration is **1.04 mol/L**.

2. Determine the pH values of the following solutions approximately.
   a) 0.1 M HNO$_3$ b) 0.1 M acetic acid (K$_A$ = 1.75 · 10^{-5} mol/L)

   c) 2 M acetic acid/1 M sodium acetate

   a) HNO$_3$ is a strong single-proton acid. Assuming full dissociation, the pH value is: $pH = -\lg c(H^+) = -\lg c(HNO_3) = -\lg 0.1 = \mathbf{1}.$
   b) Acetic acid is a very weak acid. Thus, use the approximation of almost no dissociation (obtained from mass effects law): $K_A = \frac{c(H^+)^2}{c_0(acetic\ acid)}.$ With this, pH is **2.87**.
   c) This is a buffer. Use the Henderson-Hasselbalch equation to solve this problem.
   $$pH = pK_A + \frac{c(base)}{c(corresponding\ acid)} = 4.75 + \frac{1\ M}{2\ M} = \mathbf{5.25}.$$

3. What is the basic measurement principle of a pH electrode?

   A pH electrode is a hydrogen ion-selective glass electrode. It consists of several parts with different standard solutions within these parts. By putting the electrode into a sample solution, the outer glass sphere is able to exchange sodium ions from the glass with hydrogen ions in the solution resulting in a change of potential.

Part 2 – Physical Chemistry

4. Note the second principle of thermodynamics as well as the statistical definition of entropy. What does this last equation mean?

The second law of thermodynamics introduces the entropy S. In principle, it dictates which one of all the possible processes in the system is actually realized.

The statistical definition is also known as Boltzman's rule: $S = k_B \cdot \ln W$ with W being the number of possibilities to realize one state. In a thermodynamic ensemble only one state is realized in the state of equilibrium because it is so much more likely than all the other ones.

5. Note the equation of Gibb's free enthalpy. The table below shows four conditions regarding changes in enthalpy ΔH and entropy ΔS. Give the conditions for a spontaneous process (ΔG < 0) according to the given criteria.

$\Delta G = \Delta H - T \cdot \Delta S$ must be < 0 in order to be spontaneous (exergonic).

Change in enthalpy	Change in entropy	Conditions for spontaneous process
exothermic (ΔH < 0)	decrease (ΔS < 0)	below a certain T
exothermic (ΔH < 0)	increase (ΔS > 0)	always
endothermic (ΔH > 0)	decrease (ΔS < 0)	never
endothermic (ΔH > 0)	increase (ΔS > 0)	above a certain T

6. Organic chemistry often deals with free rotation around sigma-bonds. Quantum mechanical calculations show that the difference in energy between staggered and eclipsed conformation of ethane is around 10 kJ/mol. At which ratio the two conformers of ethane equilibrate at room temperature (25 °C)?
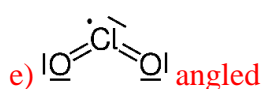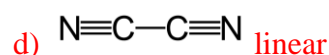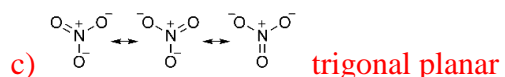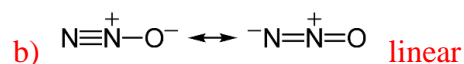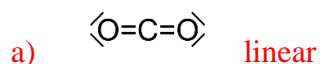
Use Boltzman's equilibrium equation for this task: $\frac{N_1}{N_0} = e^{-\frac{\Delta E}{RT}}$ with N_0 being the state with lower energy while N_1 is the state with higher energy. ΔE is the energy difference between the two states and R is the gas constant.

$\frac{N_{eclipsed}}{N_{staggered}} = \exp\left(-\frac{10000\frac{J}{mol}}{8.314\frac{J}{K \cdot mol} \cdot 298 \, K}\right) = \mathbf{0.016}$. Thus, the equilibrium lies on the staggered side (98.4 % : 1.6 %).

Part 3 – Inorganic Chemistry

7. Sketch some realistic valence bond formulas for the following molecules and predict their three-dimensional shape by applying VSEPR theory. Only take electrons of the outer shells into account.
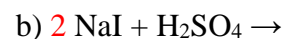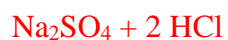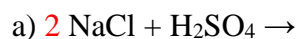
a) CO_2 b) N_2O c) NO_3^- d) NCCN e) ClO_2 f) PCl_3

a) $O=C=O$ linear

b) $N\equiv\overset{+}{N}-O^- \longleftrightarrow {}^-N=\overset{+}{N}=O$ linear

c) trigonal planar

d) $N\equiv C-C\equiv N$ linear

e) angled

f) trigonal pyramidic

8. Describe the zinc blende (ZnS) crystal structure. Refer to the lattice type and the bases. How many anions and cations can be found in a unit cell of ZnS?

The zinc blende crystal structure consists of a face centered cubic (fcc) lattice type generated by sulfide ions with 50 % of the tetrahedral gaps being occupied by zinc cations. This results in a 1:1 ratio of cations and anions. Four cations and four anions are found in a unit cell.
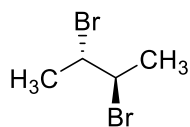
9. Give the chemical equations for the following transformations. How do the products differ?

a) $2\ NaCl + H_2SO_4 \rightarrow$ b) $2\ NaI + H_2SO_4 \rightarrow$
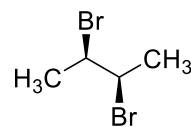
$Na_2SO_4 + 2\ HCl$ $Na_2SO_4 + 2\ HI$

HI is the stronger acid in comparison to HCl.

Part 4 – Organic Chemistry

10. Sketch (*R,S*)-2,3-dibromobutane and (*R,R*)-2,3-dibromobutane in their ecliptic and staggered conformation as Sawbuck and Newman projections respectively. Are these molecules chiral? Only the (*R,R*) conformer is chiral (no mirror plane within molecule).
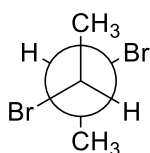

(R,S)-2,3-dibromobutane

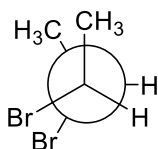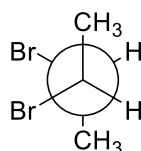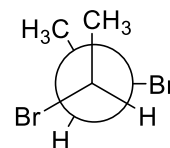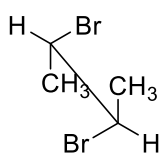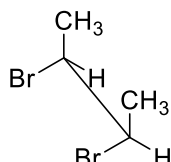(R,R)-2,3-dibromobutane
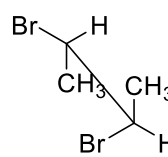
Newman projection

staggered   eclipsed
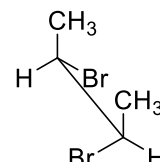
staggered   eclipsed
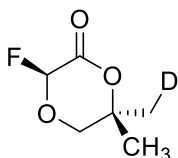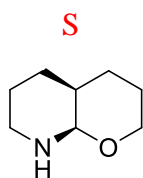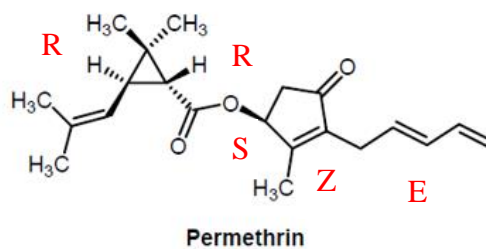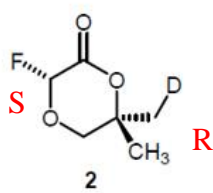
Sawsbuck projection

staggered   eclipsed

staggered   eclipsed

11. a) Determine the absolute configuration of all stereocenters (*R/S*) of the molecules given below. Please also give the relative configuration of all double bonds (*E/Z*) in **Permethrin**, an insecticide. b) Draw the enantiomer of molecule **1** and a diastereomer of molecule **2**.

1

2

Permethrin

12. Complete the following transformations if a reaction seems possible.

NaCN

S_N2

no reaction

NaOH

S_N2

Br$_2$

radical starter

NBS

radical starter

H$^+$, H$_2$O

S_N1

NaOH

S_N2

no reaction (neopentyl position)

H$_2$, Pd/C