Chemistry & Materials Science
Sample test

Module 1. Choose one correct answer (each question is worth 1 point)

1.1 Calculate the standard enthalpy of the alcohol fermentation reaction of glucose, using the enthalpies of combustion: $C_6H_{12}O_6(s) \Leftrightarrow 2C_2H_5OH\ (f) + 2CO_2(g)$.

Compare the Δ_cH values° for glucose and ethanol: $\Delta_cH°(C_6H_{12}O_6)$ = -2810 kJ/mol; $\Delta_cH°(C_2H_5OH)$ = -1371 kJ/mol.

A) -68 kJ/mol
B) +68 kJ/mol
C) -1303 kJ/mol
D) +1303 kJ/mol
Answer: A.

1.2 Use the data below to determine the order of the kinetic equation of a maltose hydrolysis reaction

initial concentration c_o mol / l	0.005	0.05	0.5
half-turn period, $t_{0.5}$, min		4.1	4.05

4.2
A) zero
B) first
C) second
D) fractional
Answer: B.

1.3 Calculate the enthalpy increase for H_2 (8 g) in a 3 l closed vessel heated from 273 K to 343 K.

A) 5820 J;
B) 9312 J;
C) 3492 J;
D) 8148 J.
Answer: D.

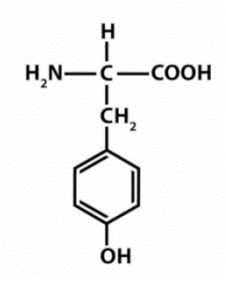
1.4 A dimer X_2 irreversibly decomposes to two molecules of X with a reaction rate constant of 0.02 s^{-1}. The initial concentration of X_2 was 0.34 mol/L. Calculate the change in the concentration of X_2 in the time interval between minutes 2 and 5 after the start of the experiment.

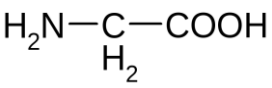
A) 0.12 mol/L;
B) 0.03 mol/L;
C) 0.54 mol/L;

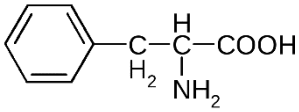
D) 0.17 mol/L.

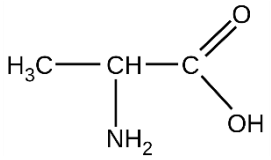
Answer: B.

1.5 The brain neuropeptide Met-enkephalin has an amino acid sequence: Tyr - Gly - Gly - Phe - Met. Which of the amino acids is not included in the structure of Met-enkephalin:

A) 

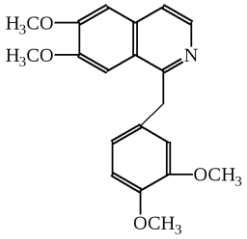
B) 

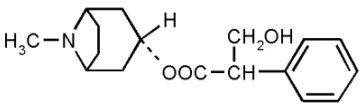
C) 

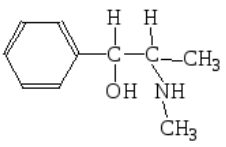
D) 

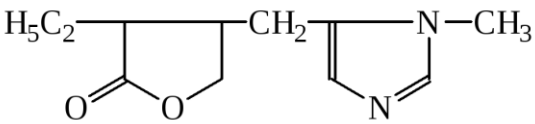
Answer: D

1.6 The isoquinoline cycle is part of the structure of a natural alkaloid

A) 

B) 

C) 



D)

Answer: A.

1.7 A galvanic cell consists of a copper cathode immersed in a 0.06 mol/L $Cu(NO_3)_2$ solution and a silver anode coated with a layer of AgCl precipitate immersed in a 0.45 mol/L NaCl solution. What is the voltage of this galvanic cell? The standard reduction potentials for reactions $Cu^{2+} + 2e^- = Cu$ and $AgCl + e^- = Ag + Cl^-$ are 0.34 V and 0.22 V respectively.

A) 0.06 V
B) 0.10 V
C) 0.56 V
D) 0.12 V

Answer: A.

1.8 Sphalerite and wurtzite

A) have the same crystal structure, but contain different impurities;
B) differ in both crystal structure and chemical composition;
C) have the same crystal structure and the same impurities, but the concentration of these impurities is different in each case;
D) are different polymorphs with the same chemical composition.

Answer: D.

1.9 A sample is an interstitial solid solution if:

A) the atoms of one component are located in the nodes of the crystal lattice of the other component (solvent);
B) the components are mutually soluble and form a homogeneous solid phase with one of the initial components preserving its crystal lattice;
C) there is no short-range and long-range order in the structure;
D) the diffraction pattern does not contain any sharp diffraction maxima.

Answer: B.

1.10 Components that neither dissolve each other in the solid state nor react with each other to produce a new compound form

A) interstitial solid solutions;
B) a chemical compound;
C) mixtures;
D) substitutional solid solutions.

Answer: C.

Module 2. There is more than one correct answer to each question (3 points are awarded for each question answered correctly)

2.1 There is a solution containing silver nitrate and potassium chloride. What TWO substances should be added in small amounts to this solution for the surface of the formed solid phase to be negatively charged?

A) calcium sulfate
B) potassium chloride
C) Barium nitrate
D) Aluminum chloride
E) Sodium nitrate

Answer: B, D.

3 points for 2 correct answers
1 point for 1 correct answer

2.2 Which TWO of the below are fixed phase interfaces?

A) methylene blue solution-air
B) methylene blue solution-benzene
C) methylene blue solution-kaolin
D) methylene blue solution-activated carbon
E) methylene blue solution-chloroform

Answer: C, D.

3 points for 2 correct answers
1 point for 1 correct answer

2.3 Which THREE of the following statements are correct?

A) The isothermal compression of an ideal gas results in a decrease in entropy.
B) The half-life of any reaction does not depend on the initial concentration of the reactant.
C) At low atmospheric pressures (at high altitudes, for example), the liquid/gas phase transition of water occurs at a temperature below 100 °C.
D) For the second-order reaction 2A → P, ln[A] depends linearly on time.
E) The rate of an elementary reaction cannot depend on the concentration of reaction products.
F) The osmotic pressure of a glucose solution is higher than that of a KBr solution with the same concentration.

Answer: A, C, E.

2.4 Complete mutual solubility of two simple substances in the solid state is possible if (choose THREE conditions):

A) these substances are similar in their mechanical properties in the solid state;
B) these substances have the same crystal lattice in the solid state;
C) the atoms of these substances are of similar sizes;

D) the elements corresponding to these simple substances are adjacent in the periodic table;
E) the elements corresponding to these simple substances have similar electronegativity values;
F) these substances have similar conductivity values.
Answer: B, C, E.

2.5 The TWO functional groups having electron-acceptor properties in relation to the benzene ring are:

A) –COOH
B) $-OC_2H_5$
C) $-NHCH_3$
D) –OH
E) $-SO_3H$

Answer: A, E.
3 points for 2 correct answers
1 point for 1 correct answer

2.6 Select TWO heterofunctional compounds that, when heated, produce a reaction of elimination:
A) CH3-CH(OH)-CH2-CH2-COOH
B) (CH3)2CH-CH(OH)-COOH
C) CH3-CH(NH2)- CH2-CH2-CH2-COOH
D) CH3-CH(OH)-CH2-COOH
E) CH3-CH(NH2)-CH2-COOH
Answer: D, E.
3 points for 2 correct answers
1 point for 1 correct answer

2.7 The melting point of silver nanoparticles is below that of the bulk phase of silver because of the size effect. Which THREE characteristics are needed to estimate the radius of silver nanoparticles if the melting point of these nanoparticles is known?
A) the surface tension of silver at the solid-gas interface;
B) the temperature and specific enthalpy of the bulk phase of silver;
C) the surface tension of silver at the liquid-gas interface;
D) the surface tension of silver at the solid-liquid interface;
E) the density of silver;
F) the melting temperature and specific melting enthalpy of the bulk phase of silver.
Answer: D, E, F.

2.8 Which THREE crystals have the same chemical composition?
A) galenit
B) sphalerit

C) wurtzit
D) zink sulfide
E) trydimite
F) pyrite
Answer: B, C, D.

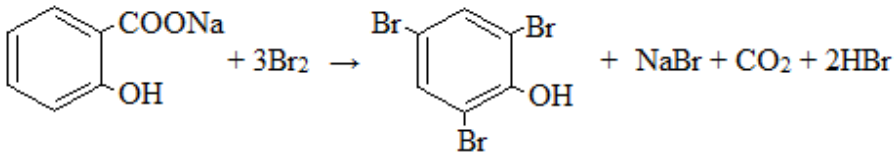
2.9 Which THREE statements are correct?
A) Enthalpy is a state function.
B) The reaction rate never depends on the concentration of reaction products.
C) Activation energy cannot be negative.
D) If the reaction enthalpy is negative, chemical equilibrium shifts towards reactants as temperature increases.
E) The liquid/gas phase transition of water always occurs at 100 °C.
F) The half-life of a second-order reaction depends on the initial concentration of the reactant.
Answer: A, D, F.

2.10 Which anode type should be used in the X-ray diffraction analysis of a Co sample to avoid secondary (fluorescent) X-ray emission? (λ_K (Co) = 1,608 Å). Choose THREE answers.
A) Fe ($\lambda_{K\alpha}$ = 1.937 Å)
B) Cr ($\lambda_{K\alpha}$ = 2.291 Å)
C) Cu ($\lambda_{K\alpha}$ = 1,542 Å)
D) Ag ($\lambda_{K\alpha}$ = 0,561 Å)
E) Mo ($\lambda_{K\alpha}$ = 0,711 Å)
F) Ni ($\lambda_{K\alpha}$ = 1,629 Å)
Answer: A, B, F.

Module 3. Tasks with a detailed answer (each correct answer is worth 12 points)

3.1 Sodium salicylate (a sodium salt of orthooxybenzoic acid) belongs to the group of non-narcotic analgesics. It has antipyretic and anti-inflammatory effects. Reverse bromatometric titration is used to quantify the content of sodium salicylate in the preparation. A sample of the preparation weighing 0.075 g is placed in a 50 ml volumetric flask; water is poured into the flask to reach the mark. Then, 25.0 ml of potassium bromate solution with a concentration of 0.033 mol/l, 1 g of potassium bromide (excess) and 10 ml of 2 M hydrochloric acid solution are added to the solution, which is left for 15 minutes. After that, 1 g of potassium iodide (excess) is added, and the solution is left in a dark place for 10 minutes. The released iodine is titrated with a solution of sodium thiosulfate with a concentration of 0.200 mol/l until the solution discolors. In the titration, 11.20 ml of sodium thiosulfate are used. Write reaction equations for this method of quantitative sodium salicylate determination (during bromination, salicylic acid decarboxylation occurs). Calculate the mass fraction (in %) of sodium salicylate in the preparation (all the reactions are quantified).
Solution:

$KBrO_3 + 5KBr + 6HCl \rightarrow 3Br_2 + 6KCl + 3H_2O$



$Br_2 + 2KI \rightarrow I_2 + 2KBr$

$I_2 + 2Na_2S_2O_3 \rightarrow 2NaI + Na_2S_4O_6$

Method 1

$v(KBrO3_3) = 25 \cdot 0.033 = 0.825$mmol => $v(Br_2) = 3 \cdot 0.825 = 2.475$ mmol

$v(Na_2S_2O_3) = 11.2 \cdot 0.2 = 2.24$ mmol

$v(Br_{2\ excess}) = v(I_2) = 2.24 / 2 = 1.12$ mmol

$v(Br_{2\ per\ salicylate}) = 2.475 - 1.12 = 1.355$ mmol

$v(C_7H_5O_3Na) = 1.355 / 3 = 0.452$ mmol

$m(C_7H_5O_3Na) = 0.452 * 160 = 72.27$ mg $= 0.07227$ g

$\omega(C_7H_5O_3Na) = 0.07227/0.075 = 0.964$ (96.4%)

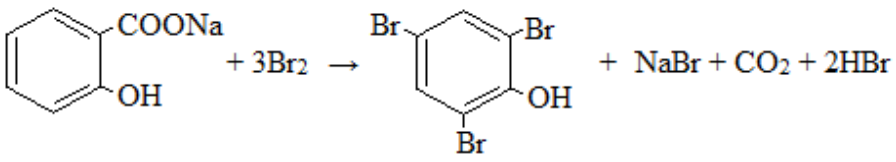
Method 2

$$\omega(C_7H_5O_3Na) = \frac{[V(KBrO_3) - V(Na_2S_2O_3)] \cdot T}{m_{(preparation)}} \cdot 100$$

$$T = \frac{c(Na_2S_2O_3) \cdot M(1/6C_7H_5O_3Na)}{1000}$$

$T = 0.2 \cdot 26.67 : 1000 = 0.00533$ g / ml

$\omega(C_7H_5O_3Na) = (25 - 11.2) \cdot 0.00533 \cdot 100 : 0.075 = 96.4\%$

Assessment criteria (other formulations are possible, as long as the answer remains correct)	Points
ANSWER ELEMENTS The equation of the chemical reaction has been written: $KBrO_3 + 5KBr + 6HCl \rightarrow 3Br_2 + 6KCl + 3H_2O$  $Br_2 + 2KI \rightarrow I_2 + 2KBr$	4

$I_2 + 2Na_2S_2O_3 \rightarrow 2NaI + Na_2S_4O_6$ $v(KBrO_3) = 25 \cdot 0.033 = 0{,}825$ mmol => $v(Br_2) = 3 \cdot 0{,}825 = 2.475$ mmol $v(Na_2S_2O_3) = 11.2 \cdot 0.2 = 2.24$ mmol $v(Br_{2\ excess}) = v(I_2) = 2.24/2 = 1.12$ mmol $v(Br_{2\ salicylate}) = 2.475 - 1.12 = 1.355$ mmol $v(C_7H_5O_3Na) = 1.355/3 = 0.452$ mmol $m(C_7H_5O_3Na) = 0.452 \cdot 160 = 72.27$ mg = 0.07227 g $\omega(C_7H_5O_3Na) = 0.07227/0.075 = 0.964$ (96.4%)	6 2
The answer is correct and complete; it contains all the above elements.	12
The reaction equations have been written.	4
A mistake has been made in one of the above elements, but it has not affected the solution.	10
Errors have been made in two of the above elements.	6
Mistakes have been made in three elements.	0
Maximum score	12

3.2 At elevated temperatures, CO reacts with water vapor according to the following equation:

$$CO\,(g) + H_2O\,(g) = H_2\,(g) + CO_2\,(g)$$

The thermodynamic data for reactants and reaction products at 298 K are given below:

Compound	CO (g.)	H_2O (g.)	H_2 (g.)	CO_2 (g.)
$\Delta_f H°_{298}$, **kJ/mol**	–110.5	–241.8	?	–393.5
$S°_{298}$, **J/(mol·K)**	197.6	188.7	130.5	213.7
$C_p°_{298}$, **J/(mol·K)**	29.14	33.61	28.83	37.11

Calculate the partial pressure of CO (bar) at chemical equilibrium at 850 °C. Initially, the system consisted of CO (partial pressure 1.00 bar) and H_2O (partial pressure 2.00 bar). The reaction occurs under constant pressure. Assume that the heat capacity does not depend on temperature.
Provide a detailed solution. Enter the answer rounded to two decimal places (e.g. 0.66 bar).
***Solution*.**
Since hydrogen is a simple substance, its standard enthalpy of formation at 298 K is zero. Let us find the standard enthalpy of reaction at 298 K:

$$\Delta_r H^0{}_{298} = 0 - 393{,}5 + 110{,}5 + 241{,}8 = -41{,}2\ kJ/mol$$

The change in entropy of this reaction at 298 K is:

$$\Delta_r S^0{}_{298} = 130{,}5 + 213{,}7 - 197{,}6 - 188{,}7 = -42{,}1\ J/(mol \cdot K)$$

The change in the heat capacity in this reaction is as follows:

$$\Delta_r C^0{}_{p,298} = 28{,}83 + 37{,}11 - 29{,}14 - 33{,}61 = 3{,}19\ J/(mol \cdot K)$$

Thus, the standard enthalpy of the reaction at 850°C will be:

$$\Delta_r H^0{}_{1123} = -41{,}2 + 3{,}19 \cdot 10^{-3} \cdot (1123 - 298) = -38{,}6\ kJ/mol$$

The tandard enthalpy of the reaction at 850°C is:

$$\Delta_r S^0{}_{1123} = -42{,}1 + 3{,}19 \cdot ln\left(\frac{1123}{298}\right) = -37{,}9\ J/(mol \cdot K)$$

The change in the Gibbs free energy:

$$\Delta_r G^0{}_{1123} = -38{,}6 + 37{,}9 \cdot 10^{-3} \cdot 1123 = 3{,}96\ kJ/mol$$

The equilibrium constant:

$$K_p = exp\left(\frac{-3960}{8{,}314 \cdot 1123}\right) = 0{,}6545$$

If the *x* bar of CO has reacted,

$$K_p = \frac{x^2}{(1-x)(2-x)} = \frac{x^2}{2 - 3x + x^2} = 0{,}6545$$
$$1{,}528x^2 = 2 - 3x + x^2$$
$$0{,}528x^2 + 3x - 2 = 0$$
$$D = 9 + 4 \cdot 2 \cdot 0{,}528 = 13{,}22$$
$$x = \frac{-3 + \sqrt{13{,}22}}{2 \cdot 0{,}528} = 0{,}603$$

Hence, the partial pressure of CO at equilibrium will be:

$$P_{CO} = 1 - 0{,}603 = 0{,}397\ `$$

Answer: 0.40 bar.

The standard enthalpy of the reaction at 298 K is worth 1 point.
The change in entropy at 298 K is worth 1 point.
The change in heat capacity is worth 1 point.
The standard enthalpy of the reaction at 1123 K is worth 2 points.
The change in entropy at 1123 K is 2 points.
The equilibrium constant is worth 2 points.

The partial pressure of CO at equilibrium is worth 3 points.
Total: 12 points.

3.3 Acetaldehyde weighing 44 g was divided into two equal portions. One part was reduced in 70% yield to obtain an ester, whilst the other was oxidized. In the esterification reaction, 15 g of an ester was obtained. Calculate the yields of the oxidation and esterification reactions if the mass fraction of acid in the mixture obtained after removing all inorganic substances is 1.85 times the mass fraction of alcohol.

Solution:

$CH_3CHO \rightarrow C_2H_5OH$

$CH_3CHO \rightarrow CH_3COOH$

$CH_3COOH + C_2H_5OH \rightarrow CH_3COOC_2H_5 + H_2O$

$\nu (CH_3CHO) = 44/44 = 1$ mol

$\nu (CH_3COOC_2H_5) = 15/88 = 0.17$ mol

$\nu (C_2H_5OH) = 0{,}5 \cdot 0{,}7 = 0.35$ mol

$m(C_2H_5OH)_{react} = 46\ (0.35 - 0.17) = 8.28$ g

$m(CH_3COOH) = 8.28 \cdot 1{,}85 = 15.32$ g

$\nu (CH_3COOH)_{react} = 15.32/60 = 0.255$ mol

$\nu (CH_3COOH)_{initial} = 0.255 + 0.17 = 0.425$ – excess

$\eta_1 = 0.425/0{,}5 = 0{,}85$ (85%)

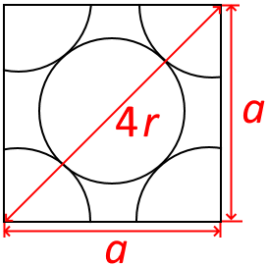
$\eta_2 = 0.17/0.35 = 0.486$ (48.6%)

Assessment criteria (other formulations are possible, as long as the answer remains correct)	Points

ANSWER ELEMENTS: The equation of the chemical reaction has been written: $CH_3CHO \rightarrow C_2H_5OH$ $CH_3CHO \rightarrow CH_3COOH$ $CH_3COOH + C_2H_5OH \rightarrow CH_3COOC_2H_5 + H_2O$ $v\ (CH_3CHO) = 44/44 = 1$ mol $v\ (CH_3COOC_2H_5) = 15/88 = 0.17$ mol $v\ (C_2H_5OH) = 0.5 \cdot 0.7 = 0.35$ mol $m(C_2H_5OH)_{вступ} = 46\ (0.35 - 0.17) = 8.28$ g $m(CH_3COOH) = 8.28 \cdot 1.85 = 15.32$ g $v\ (CH_3COOH)_{вступ} = 15.32/60 = 0.255$ mol $v\ (CH_3COOH)_{исх} = 0.255 + 0.17 = 0.425$ – excess $\eta_1 = 0.425/0{,}5 = 0.85$ (85%) $\eta_2 = 0.17/0.35 = 0.486$ (48.6%)	4 6 2
The answer is correct and complete; it contains all the above elements.	12
The reaction equations have been written.	4
A mistake has been made in one of the above elements, but it has not affected the solution.	10
Errors have been made in two of the above elements.	6
Mistakes have been made in three elements.	0
Maximum score	12

3.4 A metal has a face-centered cubic crystal structure with a unit-cell parameter of 3.62 Å (Angstrom). Calculate the atomic radius of this metal (Angstrom). Enter the answer rounded to the second decimal place (e.g. 2.89). Provide a detailed solution.

Solution. In a face-centered cubic unit cell, atoms are located at vertices and centers of the faces. Face atoms and vertex atoms touch along face diagonals, so the length of a face diagonal is equal to four atomic radii (4***r***):



Let us consider the right-angled triangle formed by two edges and a face diagonal of the cube. By applying the Pythagorean theorem, we obtain the following:

$$a^2 + a^2 = (4r)^2$$
$$2a^2 = 16r^2$$
$$a = 2\sqrt{2}\,r$$
$$r = \frac{\sqrt{2}}{4}a$$

The substitution of numerical values gives:

$$r = \frac{\sqrt{2}}{4} \cdot 3.62 \approx 1.28\ (Å).$$

Answer: 1.28 Å.

The direction in which atoms touch in the structure has been determined: 2 points.
The correct right-angled triangle for the calculation of the atomic radius has been selected: 2 points.
The Pythagorean theorem for the right-angled triangle has been used correctly: 2 points.
The correct expression for calculating the atomic radius has been obtained: 4 points.
The atomic radius has been calculated correctly: 2 points.
Total: 12 points.

3.5 Use Vegard's law to calculate the unit cell parameter in Å for the four-component solid solution $A_xB_yC_{1-y}D_{1-x}$ if x = 0.2, y = 0.4; the unit cell parameters of binary compounds composing the solution are as follows: a_{AB} = 5.5 Å, a_{AC} = 6.1 Å, a_{DB} = 4.2 Å, a_{DC} = 7.4 Å. Give the answer rounded to one decimal place. Provide a detailed solution.

Solution. The solid solution $A_xB_yC_{1-y}D_{1-x}$ consists of the following binary compounds: AB, AC, DB, and DC. According to Vegard's law, the unit cell parameter for the four-component solid solution a (x, y) can be expressed as the sum of unit cell parameters of constituent binary compounds weighted with the corresponding stoichiometric coefficients of components a_{AB}, a_{AC}, a_{DB}, and a_{DC}:

$$a\,(x, y) = xy a_{AB} + x(1-y)a_{AC} + y(1-x)a_{DB} + (1-x)(1-y)a_{DC}$$

By using the numerical values of the parameters, we obtain:

$a = 0.2 \cdot 0.4 \cdot 5.5 + 0.2 \cdot (1 - 0.4) \cdot 6.1 + 0.4 \cdot (1 - 0.2) \cdot 4.2 + (1 - 0.2) \cdot (1 - 0.4) \cdot 7.4 = 6.1$ (Å).

Answer: 6.1 Å

The expression corresponding to Vegard's law has been written correctly: 8 points.
The unit cell parameter has been calculated correctly: 4 points.
Total: 12 points.