

CHEMISTRY: ART, SCIENCE, FUN



THEORETICAL  
EXAMINATION  
ANSWER SHEETS

JULY 20, 2007  
MOSCOW, RUSSIA

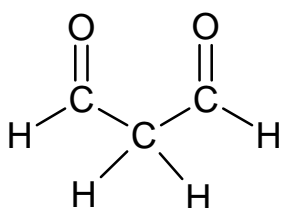
Official English version.

Problem 1	Name: _____	Quest.	1.1	1.2	2.1	3.1	3.2	3.3	3.4	Tot	Points
		Student code: _____	Marks	3	3	2	4.5	2	4	6	24.5

**1.1.1 Structures:**

Propanedial
1 <sup>st</sup> isomer
2 <sup>nd</sup> isomer

**1.1.2 Circle the acidic hydrogen atom**



*The acidity of propanedial is caused by*

- the stability of a carbanion due to conjugation with two carbonyl groups
- weakness of C–H bond in a carbonyl group
- hydrogen bonds between two propanedial molecules

The correct answer \_\_\_\_\_

**1.2.1 The structures corresponding to minima on energy curve:**

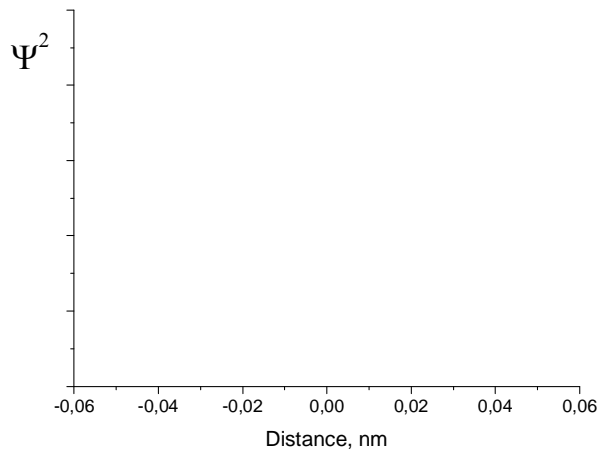
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<b>Problem 1</b>	Name: _____	Quest.	1.1	1.2	2.1	3.1	3.2	3.3	3.4	Tot	Points
	Student code: _____	Marks	3	3	2	4.5	2	4	6	24.5	7

### 1.3.1 The probability density

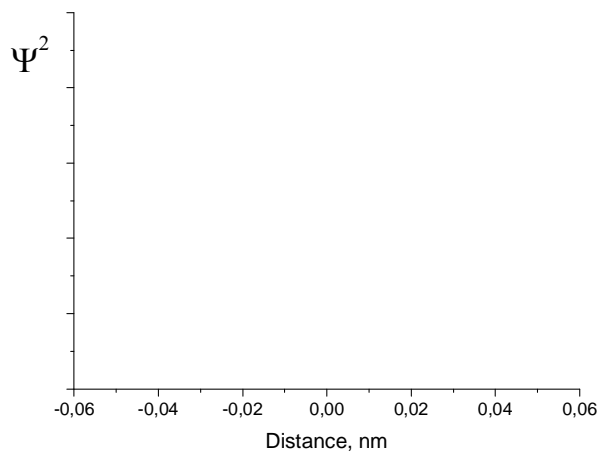
(a)  $t = 0$

$$\Psi^2(x, 0) =$$



(b)  $t = \pi/(2\omega)$

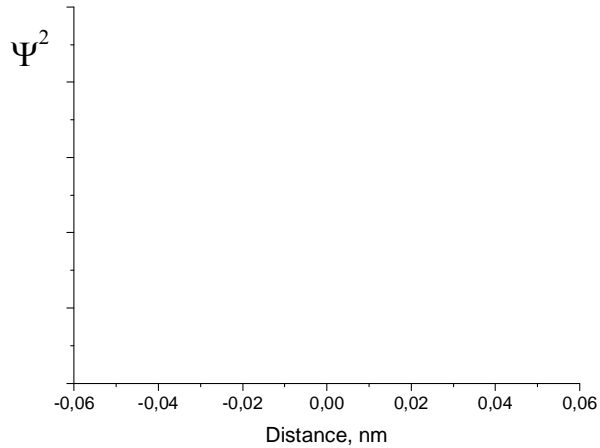
$$\Psi^2\left(x, \frac{\pi}{2\omega}\right) =$$



<b>Problem 1</b>	Name: _____	Quest.	1.1	1.2	2.1	3.1	3.2	3.3	3.4	Tot	Points
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(c)  $t = \pi/\omega$

$$\Psi^2\left(x, \frac{\pi}{\omega}\right) =$$



### 1.3.2

The probability of finding the proton in the left well = \_\_\_\_\_

### 1.3.3 The time of proton transfer

Your work:

$t =$

*The proton mean speed*

Your work:

$v =$

### 1.3.4 The uncertainty of proton position

$\Delta x =$

<b>Problem 1</b>	<b>Name:</b> _____	Quest.	1.1	1.2	2.1	3.1	3.2	3.3	3.4	Tot	Points
	<b>Student code:</b> _____	Marks	3	3	2	4.5	2	4	6	24.5	7

*The minimal uncertainty of proton velocity*

Your work:

$\Delta v =$

- Proton is a rather heavy particle, and its tunneling in malonaldehyde can be described in classical terms of position and velocity
- Proton tunneling is a purely quantum effect; it cannot be described in classical terms
- Uncertainty of proton velocity is so large that tunneling cannot be observed experimentally
- Uncertainty of proton velocity is so small that tunneling cannot be observed experimentally

The correct answer is \_\_\_\_\_

<b>Problem 2</b>	<b>Name:</b> _____	Quest.	1.1	1.2	2.1	2.2	3.1	3.2	3.3	3.4	3.5	Tot	Points
	<b>Student code:</b> _____	Marks	1	2	4	2	1	5	2	3	2	22	8

**2.1.1** *Thermodynamic data for the reaction (1):*

Your work:

$$\Delta_r G^0(1) =$$

$$K =$$

**2.1.2** *Equilibrium constant for the reaction (1) with cobalt nanoparticles:*

Your work:

$$(a) K (r = 10^{-8} \text{ m}) =$$

$$(b) K (r = 10^{-9} \text{ m}) =$$

<b>Problem 2</b>	<b>Name:</b> _____	Quest.	1.1	1.2	2.1	2.2	3.1	3.2	3.3	3.4	3.5	Tot	Points
	<b>Student code:</b> _____	Marks	1	2	4	2	1	5	2	3	2	22	8

**2.2.1** *Minimum water content in the mixture:*

Your work:

(a)  $H_2O\%$ (bulk Co) =

(b)  $H_2O\%$ (nanoparticles with  $r = 1 \cdot 10^{-9}$  m) =

**2.2.2** The correct answer is (mark the proper box):

(a)

(b)

(c)

**2.3.1** *Standard molar Gibbs function of CoO (external layer)*

$G^0(\text{CoO}, r_b) =$

**2.3.2** *Standard molar Gibbs function of Co (internal layer):*

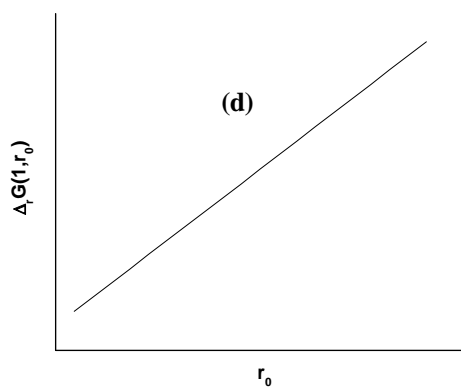
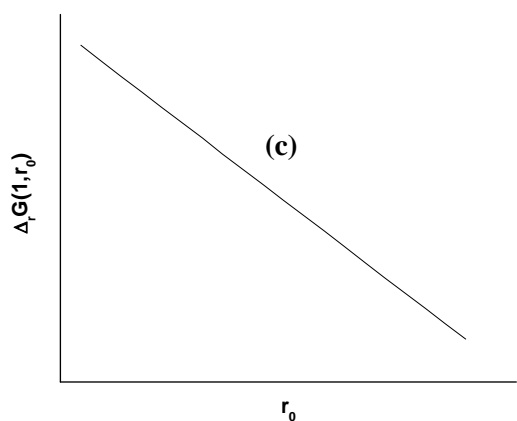
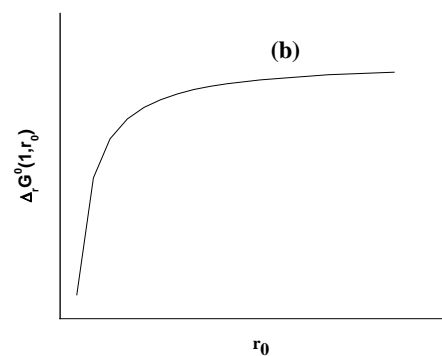
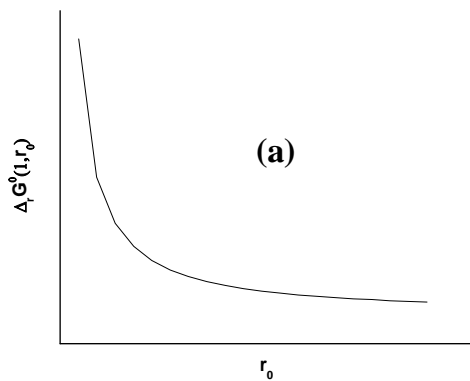
$G^0(\text{Co}, r_a, r_b) =$

**2.3.3** *Standard Gibbs energy for the reaction (1) with the double-layered nanoparticles*

$\Delta_r G^0(l, r_a, r_b) =$

Problem 2	Name: _____	Quest.	1.1	1.2	2.1	2.2	3.1	3.2	3.3	3.4	3.5	Tot	Points
	Student code: _____	Marks	1	2	4	2	1	5	2	3	2	22	8

2.3.4. Plot  $\Delta_r G^0(1, r_0)$  vs.  $r_0$



The correct plot is (mark the proper box):

(a)       (b)       (c)       (d)

2.3.5 The correct answer is (mark the proper box):

(a)       (b)       (c)



<b>Problem 3</b>	<b>Name:</b> _____	Quest.	1.1	1.2	2.1	2.2	3.1	4.1	Tot	Points
	<b>Student code:</b> _____	Marks	2	4.5	4	3	3	3	19.5	7

**3.1.1** *The overall reaction equation*

*The kinetic equation for X*

$$\frac{d[X]}{dt} =$$

**3.1.2** *The rate equation*

Your work:

$$\frac{d[P]}{dt} =$$

*Reaction orders:*

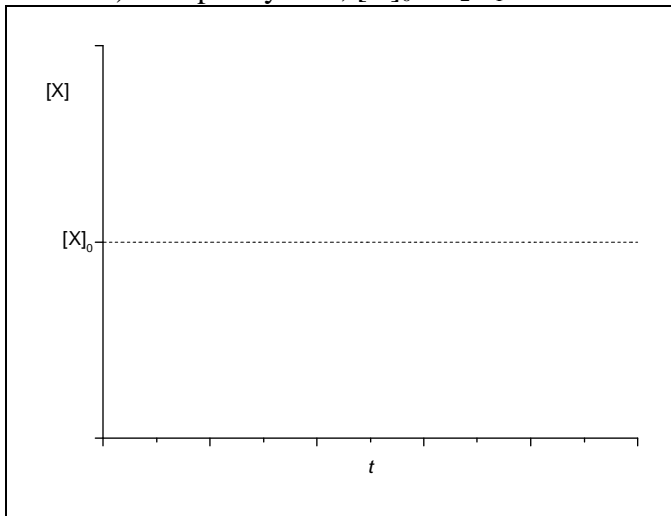
with respect to B (i): \_\_\_\_\_

with respect to D (ii): \_\_\_\_\_

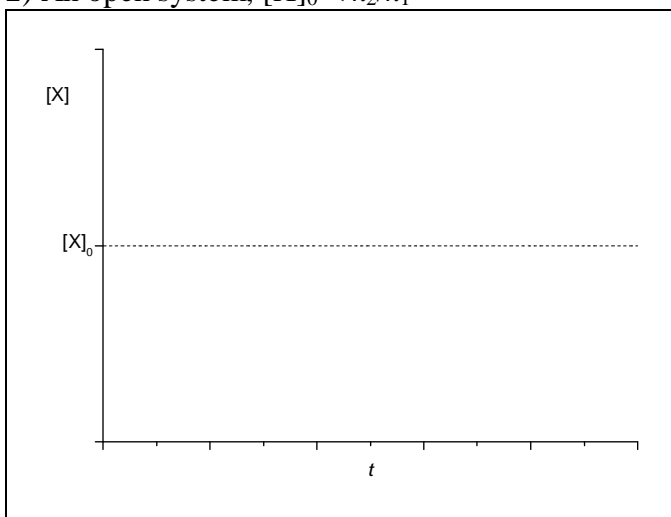
overall (iii): \_\_\_\_\_

<b>Problem 3</b>	Name: _____	Quest.	1.1	1.2	2.1	2.2	3.1	4.1	Tot	Points
	Student code: _____	Marks	2	4.5	4	3	3	3	19.5	7

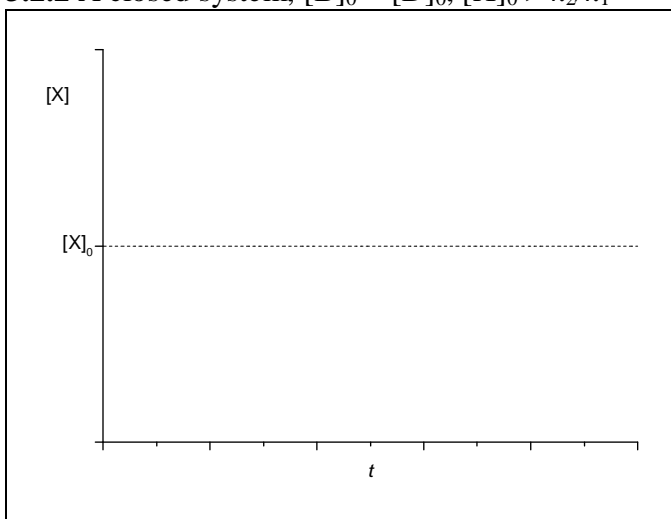
**3.2.1** 1) An open system,  $[X]_0 > k_2/k_1$



2) An open system,  $[X]_0 < k_2/k_1$



**3.2.2** A closed system,  $[B]_0 = [D]_0$ ,  $[X]_0 > k_2/k_1$



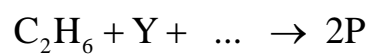
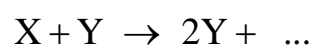
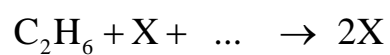
<b>Problem 3</b>	Name: _____	Quest.	1.1	1.2	2.1	2.2	3.1	4.1	Tot	Points
	Student code: _____	Marks	2	4.5	4	3	3	3	19.5	7

### 3.3.1

X –

Y –

P –



**3.4.1** The highest possible temperature:

Your work:

$T =$

<b>Problem 4</b>	Name: _____	Quest.	1	2.1	2.2	2.3	3	4.1	4.2	4.3	Tot	Points
	Student code: _____	Marks	1	1.25	1.75	2.25	1	2	1	2.25	12.5	8

**4.1. Equation:**

**4.2.1. Calculation of the  $T$  value:**

Your work:

$$T = \text{_____} \text{ mg/mL}$$

**4.2.2. Calculation of the  $T$  value:**

Your work:

$$T = \text{_____} \text{ mg/mL}$$

**4.2.3. Calculation of the  $T$  value:**

Your work:

$$T = \text{_____} \text{ mg/mL}$$

<b>Problem 4</b>	Name: _____	Quest.	1	2.1	2.2	2.3	3	4.1	4.2	4.3	Tot	Points
	Student code: _____	Marks	1	1.25	1.75	2.25	1	2	1	2.25	12.5	8

**4.3. Equation(s):**

**4.4.1 Equation(s):**

**4.4.2. Equation:**

**4.4.3. The composition of the crystallohydrate is:**

Your work:

*Formula of the salt  $Fe_2(SO_4)_3 \cdot xH_2O$ :*                       $x =$  \_\_\_\_\_

<b>Problem 5</b>	Name: _____	Quest.	1.1	1.2	1.3	2.1	2.2	3.1	3.2	Tot	Points
	Student code: _____	Marks	5	5	10	30	10	10	5	75	7.5

**5.1.1 Structure of product D**

**5.1.2** Which class of organic compounds does **D** belong to? Check the appropriate box.

*Note!* Only one checkmark is allowed. Several checkmarks will lead to 0 marks for this question.

ketones	ethers	acetals	esters	alcohols	aldehydes	glycols
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

**5.1.3** The expected yield of **D**

The yield is equal to 85% ; lower than 85% ; greater than 85%

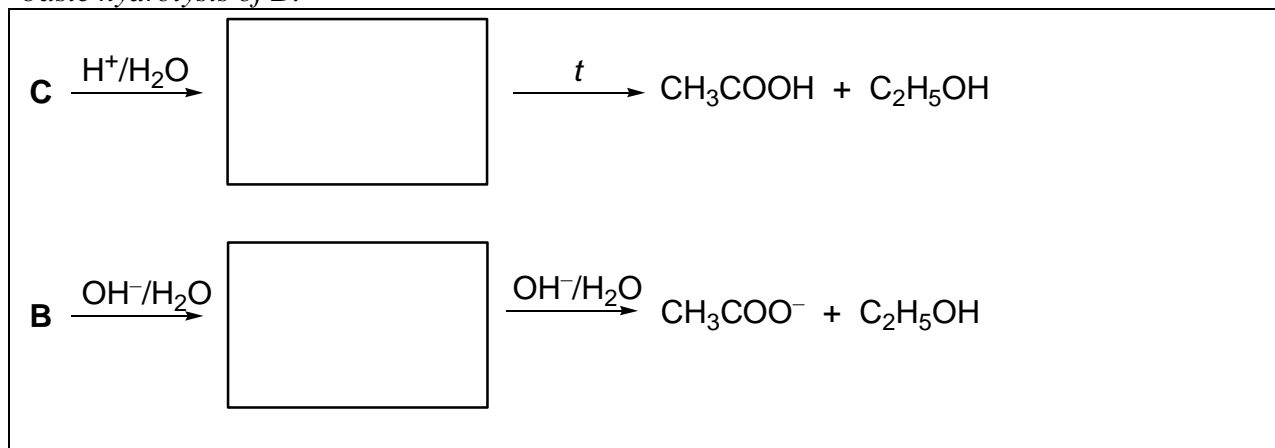
Your work:

yield =            %

**5.2.1** The structures of **A**, **B**, and **C**.

<b>A</b>	<b>B</b>	<b>C</b>

**5.2.2** Draw in the boxes intermediate compounds formed during the acidic hydrolysis of **C**, and basic hydrolysis of **B**.



<b>Problem 5</b>	<b>Name:</b> _____	Quest.	1.1	1.2	1.3	2.1	2.2	3.1	3.2	Tot	Points
	<b>Student code:</b> _____	Marks	5	5	10	30	10	10	5	75	7.5

**5.3.1** *The structure of senecioic acid and the reaction scheme leading to SA sodium salt from acetone.*

**5.3.2** *The structure of E.*

Problem 6	Name: _____	Quest.	1.1	1.2	2.1	2.2	2.3	2.4	3.1	3.2	Tot	Points
	Student code: _____	Marks	3	9	2	2	3	10	5	3	37	7

**6.1.1** *The net ionic equation accounting for the ability of LGL to set in air*

**6.1.2** *Write down the net ionic equations matching the processes enumerated in the Table. For each process check the “Yes” box if it leads to changes of pH. Otherwise check the “No” box.*

a) protonation of ortho-silicate ions leading to the formation of Si-OH groups

Reaction equation:

Yes  No

b) formation of hydrated  $[\text{SiO}_4(\text{H}_2\text{O})_2]^{4-}$  anions

Reaction equation:

Yes  No

c) polycondensation of ortho-silicate ions leading to the formation of Si-O-Si bonds

Reaction equation:

Yes  No

**6.2** *For  $[\text{Si}_3\text{O}_9]^{n-}$  ion found in aqueous solution of silicates:*

**6.2.1** *Determine the charge (n).*

Your justification

n = \_\_\_\_\_

**6.2.2** *Determine the number of oxygen atoms bridging adjacent tetrahedra.*

Your justification

*Number of oxygen atoms = \_\_\_\_\_*

**6.2.3** *Depict the ion structure joining together several tetrahedra (1).*



<b>Problem 6</b>	<b>Name:</b> _____	Quest.	1.1	1.2	2.1	2.2	2.3	2.4	3.1	3.2	Tot	Points
	<b>Student code:</b> _____	Marks	3	9	2	2	3	10	5	3	37	7

**6.2.4** *The fragment of the layered structure joining 16 tetrahedra (1)*

Your justification

Structure

**6.3.1** *pH of 0.1 M aqueous solution of copper sulfate*

Your justification

pH = \_\_\_\_\_

**6.3.2** *Equation of a reaction between aqueous solutions of  $\text{CuSO}_4$  and sodium metasilicate (LGL)*

<b>Problem 7</b>	<b>Name:</b> _____	Quest.	1.1	1.2	2.1	2.2	2.3	2.4	2.5	Tot	Points
	<b>Student code:</b> _____	Marks	12	12	5	12	7	8.5	16	72.5	7.5

**7.1.1** A number of reaction types is listed in the table below. All reactions involved in metabolism of HMG-CoA to IPP are in the list. Choose those types of reactions which are catalyzed by **E1** and **E3** (put numbers in appropriate places).

No	Reaction type
1.	Dehydration
2.	Decarboxylation
3.	Dephosphorylation
4.	4 electron reduction
5.	Release of the reduced form of coenzyme A (CoA-SH)
6.	Monophosphorylation
7.	Oxidation of hydroxyl group as the third stage of HMG-CoA $\beta$ -oxidation cycle

**E1** \_\_\_\_\_

**E3** \_\_\_\_\_

**7.1.2** Draw the structure of **X** with stereochemical details and indicate absolute configuration (*R* or *S*) of the stereocenter.

**7.2.1** Write down the overall reaction equation for reductive ozonolysis of DAP with dimethyl sulfide used as the reducing agent.

**7.2.2** Determine molecular formula of **Y**.

Your justification

Number of carbon atoms \_\_\_\_\_

Number of hydrogen atoms \_\_\_\_\_

Molecular formula: \_\_\_\_\_

<b>Problem 7</b>	<b>Name:</b> _____	Quest.	1.1	1.2	2.1	2.2	2.3	2.4	2.5	Tot	Points
	<b>Student code:</b> _____	Marks	12	12	5	12	7	8.5	16	72.5	7.5

**7.2.3** Calculate the number of IPP and DAP molecules needed to give **Y5**.

Your justification:

Number of IPP molecules \_\_\_\_\_

Number of DAP molecules \_\_\_\_\_

**7.2.4** Draw the product of coupling reaction between one IPP molecule and one DAP molecule, subsequent reductive ozonolysis of which gives **Y1**, **Y2** and one more product, the latter containing phosphorus.

**7.2.5** Draw the structures of **Y** and **Y4** with stereochemical details.

	<b>Y4</b>
	<b>Y</b>

Problem 8	Name: _____	Quest.	1.1	1.2	2.1	2.2	2.3	3.1	3.2	3.3	3.4	Tot	Points
	Student code: _____	Marks	8	9	5	11	14	16.5	12	10	13.5	99	8

**8.1.1** Expressions for the rates:

$V_{act} =$	$V_p =$
$V_{deact} =$	$V_t =$

**8.1.2** Compare rates using operators  $\ll, \leq, \approx, \geq, \gg$

$V_{deact} \quad V_{act}$	$V_{deact} \quad V_t$
$V_{deact} \quad V_p$	

**8.2.1** Mass of the obtained polymer.

Your justification:

**m** =

**8.2.2** Degree of polymerization of the obtained polymer.

Your justification:

**DP** =



<b>Problem 8</b>	<b>Name:</b> _____	Quest.	1.1	1.2	2.1	2.2	2.3	3.1	3.2	3.3	3.4	Tot	Points
	<b>Student code:</b> _____	Marks	8	9	5	11	14	16.5	12	10	13.5	99	8

**8.3.3.** *All possible reactions of activation*

P1:

P2:

**8.3.4** *Structure of P1 and one of possible structures of P2*

P1:

P2: