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UNIVERSITY OF TASMANIA

EXAMINATIONS FOR DEGREES AND DIPLOMAS

October/November 2007

KRA114

Chemistry 1B

First and Only Paper

KRA124

Chemistry 1B (Agricultural Science)

First and Only Paper

KRA164

Chemistry 1B (Pharmacy)

First and Only Paper

Examiners: Dr Chris Evenhuis, A/Prof Brian Yates, Dr Rosanne Guijt, Dr Michael Gardiner

Time Allowed: THREE (3) hours

Instructions:

Answer ALL EIGHTEEN (18) questions. All questions are of equal mark value (12 marks per question, giving a total of 216 marks). Write all answers in this booklet. Do not write in red pen.

SECTION A – THERMODYNAMICS

Dr Chris Evenhuis

Question 1

a What is meant by the standard enthalpy of formation of a substance, ΔH_f° ?

[2 marks]

b The equation for the combustion of methane in oxygen gas is: $\text{CH}_4(\text{g}) + 2 \text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2 \text{H}_2\text{O}(\text{l})$. Useful information for this part of the question is shown in the table below.

| Substance | ΔH_f° (kJ mol ⁻¹) | c_{pm} (J K ⁻¹ mol ⁻¹) |
|---------------------|--|--|
| CH ₄ (g) | -74.81 | 35.31 |
| O ₂ (g) | 0.00 | 29.36 |
| CO ₂ (g) | -393.51 | 37.11 |
| H ₂ O(l) | -285.83 | 75.29 |

i Use Hess's Law **or** an enthalpy diagram to show that the Standard Enthalpy of Combustion, ΔH_c° for methane is equal to the sum of the standard heats of formation of the products minus the standard heats of formation of the reactants.

[3 marks]

ii Use the data supplied above to calculate ΔH_c° for methane.

[3 marks]

iii Use the data supplied to calculate ΔH_c for methane at 10.0 °C.

[4 marks]

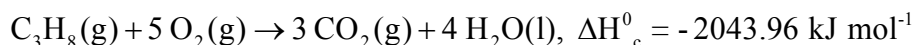
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SECTION A – THERMODYNAMICS

Dr Chris Evenhuis

Question 2

A large hall containing air at a temperature of 10 °C, a pressure of 101.5 kPa and a volume of 5000 m³ (= 5.000 x 10⁶ L) is to be heated using a portable propane gas heater. The thermochemical equation for the combustion of propane gas under standard conditions is:



The air in the hall has a composition of approximately 79.0% nitrogen and 21.0 % oxygen and by volume. For these gases, the molar heat capacities at constant pressure are:

$c_{\text{pm}}(\text{N}_2) = 29.125 \text{ J K}^{-1} \text{ mol}^{-1}$ and $c_{\text{pm}}(\text{O}_2) = 29.355 \text{ J K}^{-1} \text{ mol}^{-1}$.

a Find the amount of each gas in the room.

[3 marks]

b Show that the heat capacity of the air in the room is approximately $6.29 \times 10^6 \text{ J K}^{-1}$.

[4 marks]

c The heat energy needed to heat the air in the room by 10.0 °C is $6.29 \times 10^4 \text{ kJ}$. Calculate the mass of propane that would need to be burnt to supply the heat energy.

[5 marks]

Continued...

SECTION A – THERMODYNAMICS

Dr Chris Evenhuis

Question 3

a The isothermal expansion of a gas is a spontaneous process.

i What does this mean?

[1 mark]

ii The enthalpy change for this process is zero (0). Why is the process spontaneous?

[2 marks]

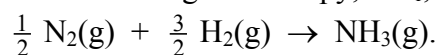
b Explain why each of the following statements is incorrect:

i the entropy of a system never decreases in a spontaneous reaction

[2 marks]

ii spontaneous processes are never endothermic

[2 marks]

c i What is the change in entropy, ΔS°_r , for the reaction:

| Compound | S° (J K ⁻¹ mol ⁻¹) |
|---------------------|--|
| NH ₃ (g) | 192.45 |
| N ₂ (g) | 191.61 |
| H ₂ (g) | 130.70 |

[3 marks]

ii Explain whether the entropy of the chemical system in part (ci) increases or decreases as you expect.

[2 marks]

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SECTION A – THERMODYNAMICS

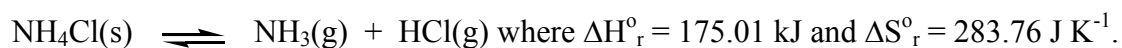
Dr Chris Evenhuis

Question 4

a Use a diagram to explain the difference between, ΔG_r° and ΔG_r

[4 marks]

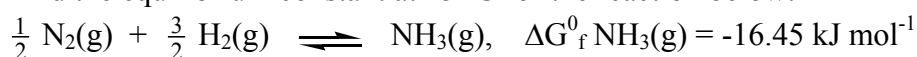
b The decomposition of ammonium chloride occurs spontaneously when the temperature of the reaction is high enough.



Determine the temperature at which the decomposition becomes spontaneous. (Identify any assumptions that you make).

[4 marks]

c i Find the equilibrium constant at 25 °C for the reaction below:



[3 marks]

ii Based on your answer to part (ci) would there be more reactants or products under these conditions.

[1 mark]

Continued...

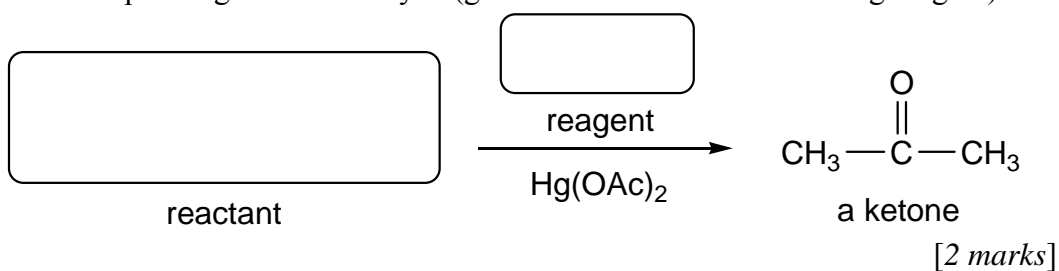
SECTION B – BIO-ORGANIC CHEMISTRY

A/Prof Brian Yates

Question 1

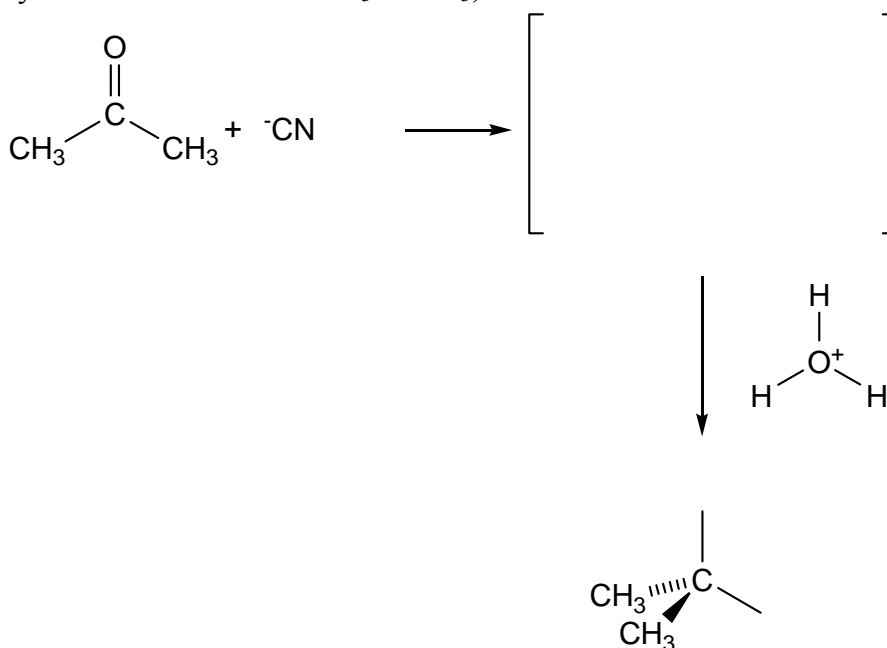
a Draw the structure of 2,2-dimethyl-3-phenylpropanal.

[4 marks]

b i Complete the following reaction for the synthesis of the ketone CH_3COCH_3 from the corresponding 3-carbon alkyne (give the reactant and the missing reagent).

ii Write down another reaction for synthesising the same ketone.

[2 marks]

c Sketch the mechanism (using curly arrows) for the nucleophilic addition reaction of cyanide with the ketone CH_3COCH_3 , shown below.

[4 marks]

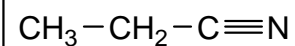
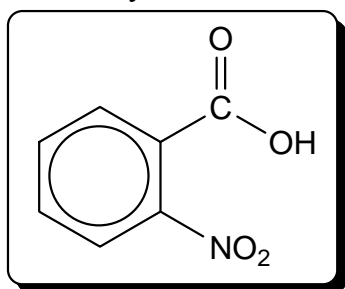
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SECTION B – BIO-ORGANIC CHEMISTRY

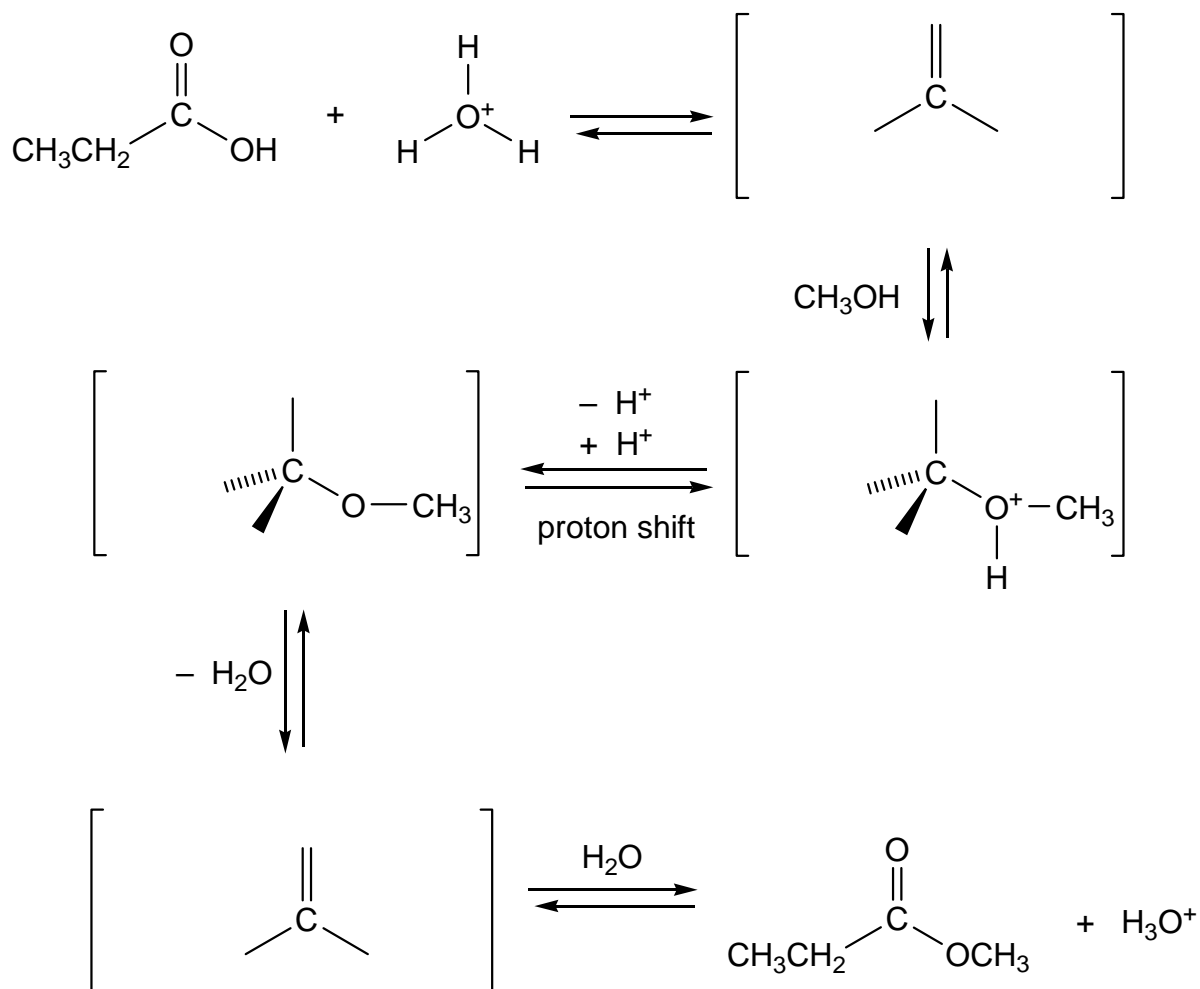
A/Prof Brian Yates

Question 2

a Give the systematic names of these compounds:



[4 marks]

b Sketch the mechanism (using curly arrows) for the Fischer esterification reaction of $\text{CH}_3\text{CH}_2\text{COOH}$ with methanol, CH_3OH , in the presence of an acid catalyst.

[8 marks]

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SECTION B – BIO-ORGANIC CHEMISTRY

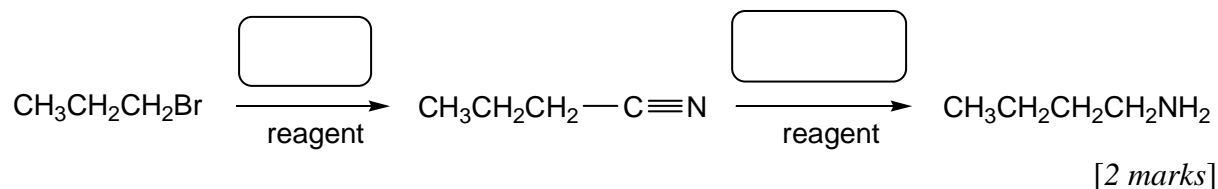
A/Prof Brian Yates

Question 3

a Draw the structures of butylamine and *N*-methyl-2-methylbutylamine.

[4 marks]

b i Complete the following reactions (give the missing reagents).



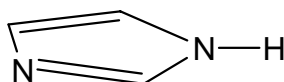
ii Is the first step substitution, elimination, oxidation or reduction?

[1 mark]

iii Is the second step substitution, elimination, oxidation or reduction?

[1 mark]

c On the picture of imidazole below, draw the orbitals in which each nitrogen has its electron lone pair, and indicate the type of hybridisation for each of these orbitals.



imidazole

[4 marks]

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SECTION B – BIO-ORGANIC CHEMISTRY

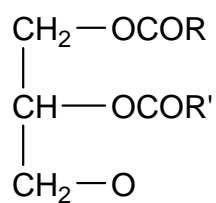
A/Prof Brian Yates

Question 4

- a Draw the general structure of a complex lipid and list three key features of the fatty acid components of the lipid.

[5 marks]

- b i Complete the general structure of the phosphoglyceride shown below:



[1 mark]

- ii Indicate the polar and non-polar ends of the molecule above.

[1 mark]

- c Explain, with a diagram, the main role of phosphoglycerides in cell membranes.

[5 marks]

Continued...

SECTION B – BIO-ORGANIC CHEMISTRY

A/Prof Brian Yates

Question 5

a What is the difference between aldose and ketose sugars?

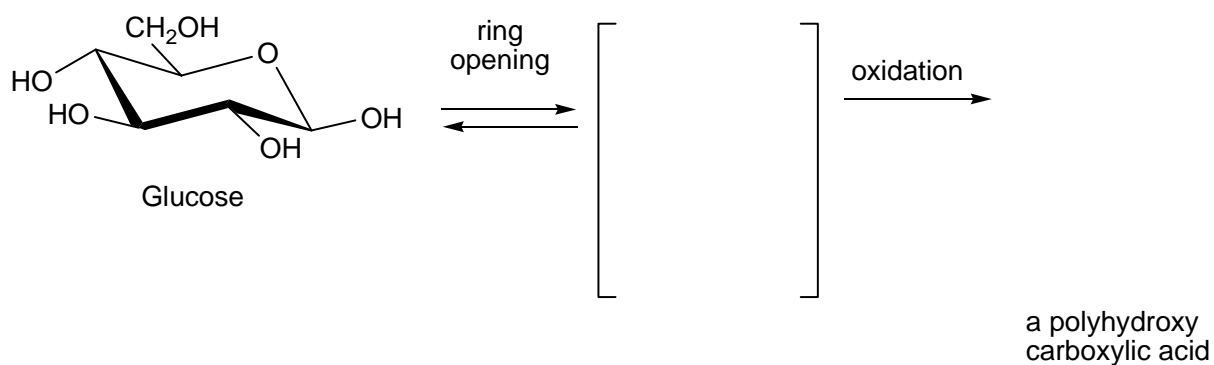
[2 marks]

b Draw the Fischer projection of a D-aldopentose sugar.

[4 marks]

c i Draw the intermediate and product of the following oxidation reaction. (Draw the structures as Fischer projections and ignore the positions of the hydroxy groups and hydrogens on the stereogenic centres.)

[4 marks]



ii What reagent could be used to carry out this oxidation? (*Hint: silver bottle!*)

[2 marks]

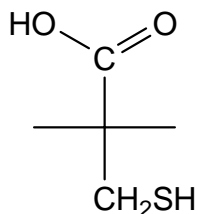
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SECTION B – BIO-ORGANIC CHEMISTRY

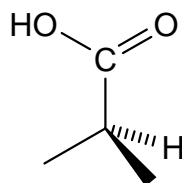
A/Prof Brian Yates

Question 6

- a Draw the Fischer projection of L-cysteine $\text{HSCH}_2\text{-CH(NH}_2\text{)-COOH}$ and then draw its corresponding three dimensional structure. Indicate if its stereochemistry is *R* or *S*.



Fischer projection



In three dimensions

Indicate the priorities of the substituents:

- COOH
- H
- CH_2SH
- NH_2

R or *S* ?

[4 marks]

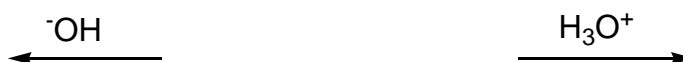
- b i Draw the zwitterion form of cysteine.

[1 mark]

- ii What does the term "zwitterion" mean?

[2 marks]

- iii Write reactions showing how the zwitterion of cysteine reacts with acid and base.



zwitterion

[2 marks]

- c i Briefly explain what is meant by the tertiary structure of a protein.

[1 mark]

- ii List two different forms of tertiary structure.

[2 marks]

Continued...

SECTION C – COLLIGATIVE PROPERTIES

Dr Rosanne Guijt

Question 1

Water has a normal boiling point of 100 °C and a normal freezing point of 0 °C. Its triple point is at 4.58 mm Hg and 0.01 °C, and above 217.7 atm (165.10^3 mm Hg) and 374 °C, water is a supercritical fluid.

- a Circle the compounds below that have a normal boiling point lower than water.

NaCl SO₂ butane (CH₃CH₂CH₂CH₃) mercury

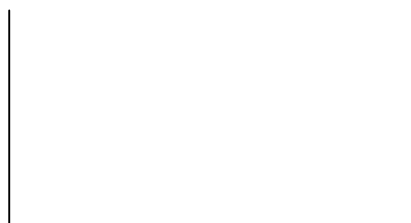
[1 mark]

- b Sketch the phase diagram for water and label the triple and supercritical point.



- c i Sketch a heating curve for water at 760 mm Hg between -30 °C and 120 °C.

[3 marks]



- ii Number the phase changes on the heating curve on part (ci). Complete the table below by naming the phases, the conversion process and indicate if the conversions are endothermic or exothermic.

[3 marks]

| phase change | initial phase | final phase | conversion process | exothermic /endothermic |
|--------------|---------------|-------------|--------------------|-------------------------|
| | | | | |

- iii 958 g of water was placed in a pan at atmospheric pressure. The system was heated and once the system reached 100 °C the energy required to evaporate all water was measured to be 2164 kJ. By calculation of the vaporisation energy, calculate the vapour pressure for water at its normal freezing point.

[2 marks]

[3 marks]

Continued...

SECTION C – COLLIGATIVE PROPERTIES

Dr Rosanne Guijt

Question 2

This question relates to colligative properties of water. For water, the normal freezing point is 0 °C and the normal boiling point is 100 °C; $K_F = 1.86 \text{ }^\circ\text{C}\cdot\text{kg/mol}$, $K_B = 0.52 \text{ }^\circ\text{C}\cdot\text{kg/mol}$. For calculation purposes, electrolytes in solution can be considered dilute and fully dissociated.

- a i It is often claimed that drinks cooled in a tub filled with a slurry of ice and water can be cooled more efficiently if table salt (pure NaCl for calculation purposes) is added to the ice slurry. Comment on the validity of this claim by calculating the freezing point of water after addition of 0.500 kg of NaCl to 4 L (4.00 kg) of water.
[3 marks]
- ii An unlabelled container containing a white crystalline solid is thought to either be sugar (sucrose, MW = 342 g/mol) or the fertiliser potash sulphur (K_2SO_4 , MW = 174 g/mol, water soluble and fully ionised in water). Discuss if measurement of the freezing point lowering of an aqueous solution containing 100 g/kg of the white solid could be used to determine the identity of the white solid.
[4 marks]
- b i It is often claimed that addition of a teaspoon of table salt (5.00 g, pure NaCl for calculation purposes) to boiling vegetables (2.00 kg water) speeds up cooking by boiling point elevation. Comment on the validity of this claim by calculating the boiling point of this solution.
[3 marks]
- ii An isotonic solution (same osmolarity as cells) contains 0.9% NaCl. Describe what will happen to vegetables if they are left in the solution described in part (bi).
[2 marks]

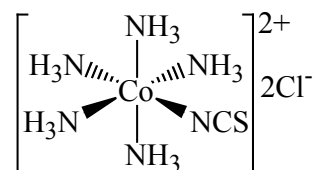
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SECTION D - COORDINATION CHEMISTRY

Dr Michael Gardiner

Question 1

a This part question refers to the following complex;



- i Determine the oxidation state of the cobalt ion in the complex. [2 marks]
- ii Give the name of the complex. [2 marks]
- iii Give the formula of the complex. [1 mark]
- iv What is the coordination number of the cobalt ion in the complex? [1 mark]
- v What is the coordination geometry of the cobalt ion in the complex? [1 mark]
- b This part question refers to the octahedral complex trisethylenediaminecobalt(III) chloride
- i Name the Lewis acid in the complex. [1 mark]
- ii What comprises the outer coordination sphere in the complex? [1 mark]
- iii Draw the structure of the complex (*do not consider more than one isomer*). [2 marks]
- iv Describe the binding arrangement of the ligands.

Continued...

SECTION D - COORDINATION CHEMISTRY

Dr Michael Gardiner

Question 2

a Draw the structures of all possible geometric isomers of the octahedral coordination complexes named below (*NOTE: marks will be deducted for duplicate structures!*);

i tetraamminedichlorocobalt(III) chloride

ii triaquatrchlorotitanium(III)

iii triamminedibromochlorochromium(III)

[8 marks]

b Use Crystal Field Theory to account for the stability of transition metal coordination complexes despite the repulsive effects of the metal-based *d* orbitals and the coordinating electron pair of the donor atoms.

[2 marks]

c i What is the name given to the type of covalent bond formed between a metal and a ligand in a coordination complex?

ii What distinguishes the metal-ligand bond discussed in part (ci) from “normal” covalent bonds?

[2 marks]

Continued...

SECTION D - COORDINATION CHEMISTRY

Dr Michael Gardiner

Question 3

- a Octahedral Cr^{3+} coordination complexes can have various colours, yet all have the same magnetic properties. Account for both of these observations.

[6 marks]

- b Is it possible to prepare a diamagnetic octahedral Mn^{3+} complex? Show your reasoning.

[6 marks]

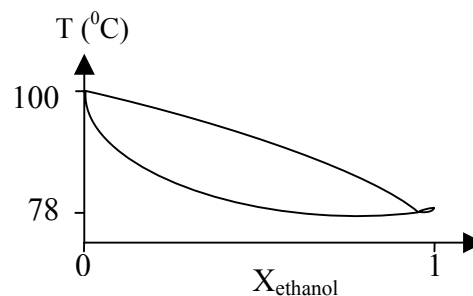
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SECTION E – SEPARATION TECHNIQUES

Dr Chris Evenhuis

Question 1

a Ethanol boils at 78.3 °C and water at 100.0 °C. A phase diagram for mixtures of water and ethanol at a pressure of 1 atm is shown in the adjacent diagram.



i Label the composition of the azeotropic mixture of water and ethanol on the X_{ethanol} mole fraction axis on the diagram.

[1 mark]

ii Use the diagram above to estimate the composition of the azeotrope.

[1 mark]

The azeotrope contains approximately _____ % ethanol.

iii Use the phase diagram to estimate the fraction of ethanol that would be present in the distillate if you start with a mixture containing 20 % ethanol and 80 % water.

[2 marks]

iv Explain why the distillate in part (iii) has a higher concentration of ethanol than the starting mixture.

[2 marks]

v Explain why an azeotrope cannot be purified by repeated simple distillation or fractional distillation.

[2 marks]

b Iodine molecules combine with iodide ions in an equilibrium process to form tri-iodide ions as shown: $\text{I}_2(\text{aq}) + \text{I}^-(\text{aq}) \rightleftharpoons \text{I}_3^-(\text{aq})$.

Briefly describe an experiment for quantitatively extracting the iodine from an aqueous mixture containing $\text{I}_2(\text{aq})$, $\text{I}^-(\text{aq})$ and $\text{I}_3^-(\text{aq})$. Briefly justify your answer.

[4 marks]

Continued...

SECTION E – SEPARATION TECHNIQUES

Dr Chris Evenhuis

Question 2

- a The insecticide DDT can be extracted from water using octanol. The partition coefficient is 6.19.
- What volume of octanol would be required for the removal of 99 % of the DDT from 100 mL of water using a single extraction?
[2 marks]
 - Calculate the % of DDT extracted from 100 mL of an aqueous solution using six repeated 20 mL extractions of octanol.
[3 marks]
 - Explain why the process of multiple small extractions is more efficient than a single large extraction.
[2 marks]
- b Ibuprofen is a weakly acidic anti-inflammatory drug, $K_a = 2.63 \times 10^{-5}$, with a partition coefficient of 25.0 when distributed between water and an organic solvent. Only the undissociated form of the drug is soluble in the organic solvent.
- Calculate the % of ibuprofen extracted from 100 mL of a 1.0 mM aqueous solution buffered to a pH of 5.00 using 25.0 mL of the organic solvent.
[3 marks]
 - To extract ibuprofen from water, would it be more efficient to use a lower pH or a higher pH for the aqueous solution? Explain your answer.
[2 marks]

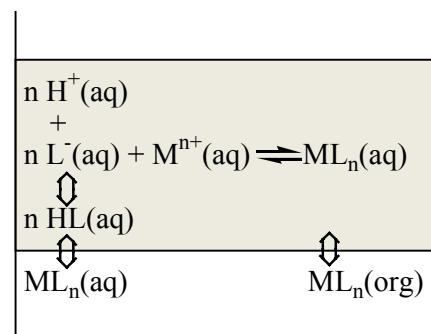
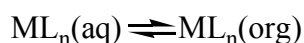
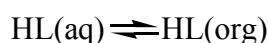
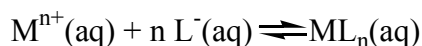
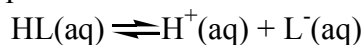
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SECTION E – SEPARATION TECHNIQUES

Dr Chris Evenhuis

Question 3

The relevant equilibria for extracting a neutral metal-ligand complex from an aqueous solution into an organic phase are shown below and in the adjacent diagram.



- a i Use the diagram above to explain the difference between the partition constant K_{pML_n} and the distribution coefficient for the metal, D .

[2 marks]

- ii Write simple expressions for K_{pML_n} and D using the diagram above.

[2 marks]

- b Under certain conditions, the distribution coefficient for the metal between the two phases in the system above is given by the expression:

$$D = \frac{K_{\text{pML}_n} \cdot K_{\text{ML}_n} \cdot (K_{\text{aHL}})^n}{(K_{\text{pHL}})^n} \cdot \frac{[\text{HL}]_{\text{org}}^n}{[\text{H}^+]_{\text{aq}}^n}$$

$\text{Cu}^{2+}(\text{aq})$ is to be extracted from an aqueous solution into an organic solvent using a weakly acidic chelating agent, HL, dissolved in the organic phase. The values for the system are: $K_{\text{pHL}} = 1.0 \times 10^4$, $K_{\text{pML}_n} = 7.0 \times 10^4$, $K_{\text{aHL}} = 5.0 \times 10^{-5}$ and $K_{\text{ML}_n} = 2.5 \times 10^{16}$.

- i Calculate the extraction efficiency when 100 mL of 1.0×10^{-6} M $\text{Cu}^{2+}(\text{aq})$ is extracted using 25 mL of organic solvent containing the chelating agent at a concentration of 1.0×10^{-3} M at pH = 3.

[5 marks]

- ii Why would the extraction be inefficient at a pH of 10? Explain your reasoning.

[3 marks]

| Section | A Thermo | B Bio-org Chem. | C Collig. Props | D Coord. Chem. | E Sep. Techs |
|---------|-------------|-----------------------|-----------------------|----------------------|--------------------|
| Q1 /12 | | | | | |
| Q2 /12 | | | | | |
| Q3 /12 | | | | | |
| Q4 /12 | | | | | |
| Q5 /12 | | | | | |
| Q6 /12 | | | | | |
| Totals | | | | | |

Grand Total

/216

SOME FUNDAMENTAL CONSTANTS

| | | |
|---|---|--|
| Avogadro Number (N) or (L) | = $6.022 \times 10^{23} \text{ mol}^{-1}$ | |
| Faraday (F) | = $96,485 \text{ C mol}^{-1}$ | |
| Boltzmann constant (k) | = $1.381 \times 10^{-23} \text{ J K}^{-1}$ | |
| Planck constant (h) | = $6.626 \times 10^{-34} \text{ J s}$ | |
| Speed of light in vacuum (c) | = $2.998 \times 10^8 \text{ m s}^{-1}$ | |
| Rydberg constant (R_H) | = $2.18 \times 10^{-18} \text{ J}$ | |
| Atomic mass unit (amu) | = $1.661 \times 10^{-27} \text{ kg}$ | |
| Gas Constant (R) | = $8.314 \text{ J K}^{-1} \text{ mol}^{-1} = 0.08206 \text{ L atm mol}^{-1} \text{ K}^{-1}$ | |
| Standard atmosphere | = $1.01325 \times 10^5 \text{ Pa} \equiv 760 \text{ torr} \equiv 760 \text{ mmHg} \equiv 1 \text{ atm}$ | |
| Kelvin/Celsius Temperature conversion: $T(\text{K}) = T(^{\circ}\text{C}) + 273.15$ | | |

SOME MATHEMATICAL RELATIONSHIPS

$$\ln(x) = y \Rightarrow x = e^y \qquad \log(x) = y \Rightarrow x = 10^y \qquad \log(x/y) = \log(x) - \log(y)$$

SOME CHEMICAL FORMULAE

General equations

$$c = \lambda \nu \qquad E = h\nu \qquad \lambda = \frac{h}{m\nu} \qquad \Delta E = R_H \left(\frac{1}{(n_i)^2} - \frac{1}{(n_f)^2} \right) \qquad pV = nRT$$

$$m_A = \frac{n_A}{m_{\text{solvent}}} \qquad [A] = \frac{n_A}{V} \qquad X_A = \frac{n_A}{n_{\text{total}}} \qquad n_A = \frac{m_A}{MW_A}$$

Kinetics related equations

For $aA + bB \rightarrow cC + dD$,

$$\text{rate} = -\frac{\Delta[A]}{a\Delta t} = -\frac{\Delta[B]}{b\Delta t} = \frac{\Delta[C]}{c\Delta t} = \frac{\Delta[D]}{d\Delta t}$$

$$= k[A]^m[B]^n$$

$$k = Ae^{-E_a/RT}$$

For $A \rightarrow$ products,

if a 1st order reaction:

$$\ln[A]_t = -kt + \ln[A]_0$$

$$t_{1/2} = -\ln(1/2) / k = \frac{0.693}{k}$$

For $A \rightarrow$ products,

if a 2nd order reaction:

$$\frac{1}{[A]_t} = kt + \frac{1}{[A]_0}$$

Equilibrium-Acid/Base related equations

For $aA + bB \rightarrow cC + dD$,

$$K_c = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

$$pH = pK_a + \log\left(\frac{[\text{base}]}{[\text{acid}]}\right)$$

$$pK_w = pK_a + pK_b = 14 = pH + pOH$$

$$K_p = K_c (RT)^{\Delta n_g}$$

$$K_w = K_a \cdot K_b = 1.01 \times 10^{-14}$$

$$= [H^+][OH^-]$$

$$pX = -\log(X)$$

$$pH = -\log[H_3O^+]$$

Thermodynamics/colligative properties related equations

$$w = mgh$$

$$w = -nRT \ln\left(\frac{V_f}{V_i}\right)$$

$$\Delta U = q + w$$

$$w = -p_{\text{ext}} \Delta V$$

$$\Delta G = -RT \ln(K)$$

$$c_{pm} = c_{vm} + R$$

$$q = n\Delta H$$

$$\Delta U = q_v = nc_{vm} \Delta T = mc_v \Delta T = C_v \Delta T$$

$$\Delta H = q_p = nc_{pm} \Delta T = mc_p \Delta T = C_p \Delta T$$

$$\Delta H = \Delta U + nR\Delta T = \Delta U + \Delta(pV)$$

$$\Delta G = \Delta H - T\Delta S$$

$$\ln(K) = -\frac{\Delta H^\circ}{RT} + \frac{\Delta S^\circ}{R}$$

$$\Delta G_r = \Delta G_r^\circ + RT \ln(Q)$$

$$\Delta G_r^\circ = -RT \ln(K)$$

$$\Delta H_r^\circ = \Delta H_r^\circ + \Delta C_p \Delta T$$

$$\ln\left(\frac{k_2}{k_1}\right) = -\frac{\Delta H}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$$

$$\ln\left(\frac{p_2}{p_1}\right) = -\frac{\Delta H_{\text{vap}}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$$

$$\Delta S = C_v \ln\left(\frac{T_f}{T_i}\right)$$

$$\Delta S_{\text{surr}} = -\frac{\Delta H}{T} = nR \ln\left(\frac{V_f}{V_i}\right)$$

$$\Delta S_{\text{tot}} = \Delta S + \Delta S_{\text{surr}}$$

$$\Pi = MRT$$

$$\Delta T_b = K_b \cdot m \cdot i$$

$$\Delta T_f = K_f \cdot m \cdot i$$

$$S_g = k_H \cdot p_g$$

$$p_{\text{solvent}} = X_{\text{solvent}} \cdot k_H$$

$$p_g = X_g \cdot p_g^\circ$$

$$p_g = X_g \cdot p_{\text{total}}$$

$$\text{rel. hum.} = p_{H_2O} / p_{H_2O}^\circ \times 100\%$$

Separation Science related equations

$$D = \frac{K_p \cdot K_a}{K_a + [H^+]_{\text{aq}}}$$

$$p = \frac{D}{D + V_{\text{aq}}/V_{\text{org}}}$$

$$q^n = \left(\frac{1}{1 + D \cdot V_{\text{org}}/V_{\text{aq}}} \right)^n$$

$$D = \frac{K_p [H^+]_{\text{aq}}}{[H^+]_{\text{aq}} + K_a}$$

$$p = 1 - q$$

$$K_p = \frac{[S]_2}{[S]_1}$$

$$q^n = \left(\frac{V_1}{V_1 + K_p \cdot V_2} \right)^n$$

$$D = \frac{K_p \cdot [OH^-]_{\text{aq}}}{K_b + [OH^-]_{\text{aq}}}$$

$$\frac{V_{\text{org}}}{V_{\text{aq}}} = \sqrt{\left(\frac{1}{D_a D_b} \right)}$$

$$F_{r,n} = \frac{n!}{r!(n-r)!} \left(\frac{1}{D+1} \right)^n \cdot D^r$$

$$D = \frac{K_{p_{ML_n}} \cdot K_{ML_n} \cdot (K_{a_{HL}})^n \cdot [HL]_{\text{org}}^n}{(K_{p_{HL}})^n \cdot [H^+]_{\text{aq}}^n}$$

$$\beta = \frac{D_1}{D_2} = \frac{K_{ML_n(1)} \cdot K_{p_{ML_n(1)}}}{K_{ML_n(2)} \cdot K_{p_{ML_n(2)}}}$$

$$K_{A,E} = \frac{[A^-][SP-E]}{[SP-A][E^-]}$$

PERIODIC TABLE OF THE ELEMENTS

(Updated from IUPAC, August 2003, <http://www.chem.qmul.ac.uk/iupac/AtWt/table.html>)

| | | | | | | | | | | | | | | | | | |
|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
| 1 H 1.0079 | | | | | | | | | | | 18 He 4.0026 | | | | | | |
| 2 Li 6.941 | 3 Be 9.0122 | | | | | | | | | | | 13 B 10.811 | 14 C 12.011 | 15 N 14.007 | 16 O 15.999 | 17 F 18.998 | 10 Ne 20.180 |
| 11 Na 22.990 | 12 Mg 24.305 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 Al 26.982 | 14 Si 28.086 | 15 P 30.974 | 16 S 32.065 | 17 Cl 35.453 | 18 Ar 39.948 |
| 19 K 39.098 | 20 Ca 40.078 | 21 Sc 44.956 | 22 Ti 47.867 | 23 V 50.942 | 24 Cr 51.996 | 25 Mn 54.938 | 26 Fe 55.845 | 27 Co 58.933 | 28 Ni 58.693 | 29 Cu 63.546 | 30 Zn 65.409 | 31 Ga 69.723 | 32 Ge 72.64 | 33 As 74.922 | 34 Se 78.96 | 35 Br 79.904 | 36 Kr 83.798 |
| 37 Rb 85.468 | 38 Sr 87.62 | 39 Y 88.906 | 40 Zr 91.224 | 41 Nb 92.906 | 42 Mo 95.94 | 43 Tc (98) | 44 Ru 101.07 | 45 Rh 102.91 | 46 Pd 106.42 | 47 Ag 107.87 | 48 Cd 112.41 | 49 In 114.82 | 50 Sn 118.71 | 51 Sb 121.76 | 52 Te 127.60 | 53 I 126.90 | 54 Xe 131.29 |
| 55 Cs 132.91 | 56 Ba 137.33 | 57-71 * | 72 Hf 178.49 | 73 Ta 180.95 | 74 W 183.84 | 75 Re 186.21 | 76 Os 190.23 | 77 Ir 192.22 | 78 Pt 195.08 | 79 Au 196.97 | 80 Hg 200.59 | 81 Tl 204.38 | 82 Pb 207.2 | 83 Bi 208.98 | 84 Po (209) | 85 At (210) | 86 Rn (222) |
| 87 Fr (223) | 88 Ra (226) | 89-103 # | 104 Rf (261) | 105 Db (262) | 106 Sg (266) | 107 Bh (264) | 108 Hs (277) | 109 Mt (268) | 110 Ds (281) | 111 Rg (272) | 112 ? (285) | | 114 ? (289) | | | | |

* Lanthanide series

| | | | | | | | | | | | | | | |
|---------------------------|---------------------------|---------------------------|---------------------------|--------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
| 57 La 138.91 | 58 Ce 140.12 | 59 Pr 140.91 | 60 Nd 144.24 | 61 Pm (145) | 62 Sm 150.36 | 63 Eu 151.96 | 64 Gd 157.25 | 65 Tb 158.93 | 66 Dy 162.50 | 67 Ho 164.93 | 68 Er 167.26 | 69 Tm 168.93 | 70 Yb 173.04 | 71 Lu 174.97 |
|---------------------------|---------------------------|---------------------------|---------------------------|--------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|

Actinide series

| | | | | | | | | | | | | | | |
|--------------------------|---------------------------|---------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
| 89 Ac (227) | 90 Th 232.04 | 91 Pa 231.04 | 92 U 238.03 | 93 Np (237) | 94 Pu (244) | 95 Am (243) | 96 Cm (247) | 97 Bk (247) | 98 Cf (251) | 99 Es (252) | 100 Fm (257) | 101 Md (258) | 102 No (259) | 103 Lr (262) |
|--------------------------|---------------------------|---------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|---------------------------|---------------------------|---------------------------|---------------------------|