(1)

Assiut university
Faculty of science
Chemistry Departement

June 2015
Time 2 hours

Final examination in **the chemistry of biomolecules 413 C**
(Carbohydrates,proteins,lipids,nucleic acids)

Answer the following questions----------------- 50 marks

<u>Question</u>1 Answer <u>five</u> only of the following-----17.5 marks

a-The Haworth formula of aldohexoses and ketohexoses

b- Complete and suggest a mechanism for the following reaction

D-Glucose+ 3PhNHNH2/heat---------------→ ?

c-By means of equations,how can you convert D-mannose to D-arabinose

d-Give the structure of compounds A,B and C in the following reactions

Lactose+Br2/H2O---------- A +H_3O^+-------------- B +C

e- What are the aldaric acids?

f- The chemical structures of cellulose and maltose

<u>Question</u> 2. Answer <u>five</u> only of the following-------------- 17.5 marks

a-Predict the product(s) resulting from the following reaction

D-glucose + MeOH/HCl/heat-----------------→?

b- Draw the structures of the following i-arabinoic acid , ii- D-erythrose

c-Synthesis of dipeptide(alanylglycine)

d-Give the structure of the amino acid results from the following reaction

CH3CHO + NH3/HCN------------→ ? + H_3O^+------------- ?

e- The dipolar ion(zwitter ion) of amino acids

f-Product of glycine with the following reagents i- HNO2, ii-EtOH/HCl/heat

<u>Question 3</u>. Answer <u>five</u> only of the following----------------- 15 marks

a-What are the neutral lipids?

b- The resemblance and difference between lecithins and cephalins

c-The structure and occurrence of glycolipids

d-Saturated fats resist rancidity more than unsaturated fats.Explain

e-Give the structure of the following i-cytosine , ii-Guanosine monophosphate iii-Adenosine

f-Formation of Ketones bodies from acetyl COA

Good luck

Prof.Dr,Sh.M.Radwan Sh. M. Radwan

(1)

Assiut University
Faculty of Science
Chemistry Department

June 2015
Time: 2 hours
(50 Marks)

Second Semester Examination for Biological Students
Subject: Analytical Chemistry (C- 460)

Answer the following questions: **(50 Marks)**

Q1) Answer Only Two of the following: **(12.5 Marks)**

a) Write on the following:

i) Limitation of argentometric titration. *ii)* Types of polarographic current.

b) *If you are provided with 0.1M CH_3COOH (100ml)* and titrated with 0.1M NaOH. Calculate the pH value: ($k_a=1.86x10^{-5}$)

i) at the beginning of the titration, *ii)* after the addition of 50 ml HCl and *iii)* at the end point.

c) Give the reason for the following:

i) Mohr method is applicable in neutral solution.

ii) Supporting electrolyte is used in the polarographic analysis.

Q2) Answer Only Two of the following: **(12.5 Marks)**

a) Define the following terms:

i) Ilkovic equation. *ii)* Buffer solution.

b) Calculate the diffusion current for the reduction of $5x10^{-5}$ Zn^{+2} which has diffusion coefficient $0.72x10^{-5}$ cm. sec. m = 15mg/sec. and t= 4sec/drop.

c) Write on the following:

i) The applications of potentiometric titration.

ii) Limitation of volumetric precipitation titration reaction.

Q3) Answer Only Two of the following: **(12.5 Marks)**

a) Complete:

i) The indicator in Mohr method is ----- , while in Volhard method the indicators are--------- and in Fajan method the indicators are ---------- ----.

ii) The half wave potential is------------.

b) During the titration of 100 ml 0f HCl (1N) using NaOH (1N) , Calculate the pH

i) before the titration, *ii)* after the addition of 50 ml NaOH,

iii) at the end point and *iv)* after the addition of 110 ml NaOH.

c) Define Beer Labert relationship. Calculate the absorbtivity (a) for a solution contains 4.5 ppm of a coloured species. It is found to have an absorbance of 0.3 nm at 530 nm in a 2cm cell.

Q4) Answer Only Two of the following: **(12.5 Marks)**

a) Define the following terms:

i) Standard hydrogen electrode. *ii)*The oxidizing agent and the reducing agent.

b) Show how you can use polarographic technique in qualitative and quantitative analysis.

c) Write on the following:

i) Determination of the equivalent point in potentiometric titration. (Two only).

ii) Electrochemical cell.

---------------------------------**Good Luck**-------------------------------

Examiner: Prof.Dr. ***Azza M.M.Ali***

Assiut University
Faculty of Science
Chemistry Department

(1)

Date: June 2015
Time allowed: Two hours.

Final Examination of Chemical Instrumental Analysis Course (C-445)

Subject: Final Exam of (C-445)

Students: Fourth level students, Faculty of Science

Section (I)

Answer the following questions:

1) Write on **Only Two** of the following: (12.5 Marks)

a) i- Ilkovic Equation.

ii- Calculate the diffusion current that would be expected from the reduction of 2.00×10^{-3} M Pb^{2+} if the diffusion coefficient of Pb^{2+} is 1.01×10^{-5} cm^2/sec and the mercury drop characteristics are m = 1.90 mg/sec and t= 3.47 sec/ drop.

iii- An unknown solution containing lead gives a diffusion current of 11.7 μ A with the same drop characteristics as in (ii), what is the [Pb2+] in this solution.

b) Application of masking reagents in chemical analysis.

c) Write briefly on the analytical separation by ion exchange.

2) Write on **Only Two** of the following: (12.5 Marks)

a) Stripping voltammetry.

b) i- Solvent extraction technique in chemical analysis.

ii- A substance X has a distribution coefficient of 3.7 between water and carbon tetrachloride CCl_4, calculate the concentration of X remaining in the aqueous phase after extraction of 100 ml of 1.00×10^{-3} M, X with the following quantities of CCl_4 : (a) 100 ml , (b) two 50 ml portions , (c) five 20.0 ml portions.

c) Differential pulse and square wave voltammetry.

Section (II)

Answer **Four** questions only: (25 Marks)

1) Describe the absorption phenomena taking place in the far-infrared, mid-infrared and visible – ultraviolet regions of the spectrum.

2) Write briefly on:

a) Isosbestic point. b) Continuous variation method.

3) A solution containing 4.48 ppm $KMnO_4$ has a transmittance of 0.309 in a 1-cm cell at 520 nm. Calculate the molar absorptivity of $KMnO_4$. (At.Wt K= 39.1, Mn =54.94, O = 16)

4) Give the theoretical bases of spectrophotometric quantification of binary mixtures.

5) At a wavelength of 356 nm, the molar absorptivity of a phenolic compound in 0.1 M HCl is 400 and in 0.2 M NaOH is 17000. determined in pH 9.5 buffer, the molar absorptivity is 9800. Calculate the pKa.

Examiners: Section (I) Prof. Dr. Mahmoud A. Ghandour.
Section (II) Prof. Dr. Hassan Sedaira.

اختبار نهاية الفصل الثاني

2014/2015

في

علوم الليزر وتطبيقاتة

(472 ف)

(١)

كلية العلوم

جامعة أسيوط

التاريخ:الأثنين1/6 /2015

قسم الفيزياء

الفرقة : الرابعة – نظام الساعات المعتمدة

شعبة : الفيزياء/الكيمياء

الزمن ثلاث ساعات

ملحوظة : لكل سؤال 12.5 درجة

أجب عن **أربعة** أسئلة فقط مما يأتي:

السؤال الأول:

أكتب مقالة علمية تاريخية عن خصائص الضوء – كمقدمة لفهم مبادئ الليزر؟

السؤال الثاني:

أ) عرف المفاهيم العلمية التالية:

قلب التعداد – الأتزان الحراري – الوسط الفعال لليزر. (كل فقرة 1.5 درجة)

ب) تكلم عن خصائص معاملات أينشتين لفهم كيفية الأنبعاث التلقائي والأنبعاث المرغم؟ (8 درجات)

السؤال الثالث:

أ) تكلم عن طرق الضخ الليزري – مع التوضيح بالرسم فقط – الليزرات المتعددة المستويات؟ (8 درجات)

ب) أستخدم جهاز ليزر طول أنبوبته 150مم، وكان معامل الكسب لمادته الليزرية 0.0005 سم$^{-1}$. فأذا كانت إحدي مرآتيه عاكسة للضوء بنسبة 100%، فكم يجب أن تكون إنعكاسية المرآة الأخري؟ (4.5 درجة)

السؤال الرابع:

أ) صف ميكانيكية آلية للحصول علي شعاع ليزرالياقوت (Ruby Laser) مع التوضيح بالرسم فقط – مستويات الطاقة في هذه الحاله؟ (8 درجات)

ب) إحسب التعداد النسبي لمستويين الطاقة في ليزر الياقوت عندما يكون هناك إنبعاث فوتوني بينهما ذو طول موجي 6928 أنجشتروم ، وبفرض أن درجة الحرارة للنظام 18 كيلفن؟ (4.5 درجة)

السؤال الخامس:

أ) أكتب باختصار -: مميزات وخصائص شعاع الليزر وأهم التطبيقات العملية له؟ (كل فقرة 1.5 درجة)

ب)إستنتج – باستخدام المعادلات الرياضية الفيزيائية – الشرط الحرج للحصول علي مضخم شعاع الليزر؟ (8 درجات)

ملحوظة: إستخدم الثوابت العلمية التالية – إذا لزم الأمر:

$h = 6.6 \times 10^{-34}$ J sec. , $k = 1.38 \times 10^{-23}$ J K^{-1} , $c = 3 \times 10^{8}$ m sec^{-1}

إنتهت الأسئلة – مع أطيب التمنيات بالتوفيق ،،،،،،،،،،،،،،،،،،،،،،

(1)

Assiut University June 2015
Faculty of Science
Department of chemistry Time: 3 hrs

Final Exam : Inorg.Chem. 4 (422C) for 4th level chemistry students.

Answer the following questions:

1- A) Complete the following sentences with the correct choice : (10 marks)

(i) The formation constants for metal complexes correlate well with ...... basicity if steric factors considered. (Arrhenius - Bronsted - Lewis)

(ii) Non- chelate complex formation results in .... of the independent molecules. (increase - decrease- no net charge)

(iii) If ..... is strong σ donor or - π acceptor, it greatly accelerates substitution of a ligand that is trans to itself .(entering group- leaving group- spectator ligand).

(iv) It is very difficult to distinguish between A and Ia because the composition of the activated complex is .....(unknown- unstable- the same)

(v) The .... mechanism plays a central role in octahedral substitution. (associated- dissociated - interchange)

(vi) In the Eigen-Wilkins mechanism ....complex is formed. (activated- encounter- intermediate).

(vii) Low π * electron density on the metal ion facilitates ....substitution reaction in octahedral complexes. (associative – dissociative)

(viii) In interchange mechanism of substitution in square planar complexes, the intermediate persists..... time than in the associative mechanism. (longer- shorter)

(ix) Substitution reaction of hexaaquo Ni(II) complex is considered as a model for Id reaction with ......response to the nucleophilicity of the entering group. (high- low –very low)

(x) The equilibrium constants favors the encounter if the reactants are ...... and oppositely charged (small- large).

(B) Answer <u>ONE ONLY</u> of the following : (2.5marks)

(i) Define a) The nucleophilic discrimination factor.
b) The nucleophilicity parameter.

(ii) Give the reason for :

a) The anomalous low value of K_3/K_2 for the halogeno Hg (II) complex.
b) The chiral form of the complex $[CoCl_2(bn)_2]^+$ hydrolyzes more slowly than the achiral form. (bn =2,3-butanediamine)

2- A) Put (√) or (X) in front of each of the following : (10 marks)

(i) The order of Irving –Williams series is insensitive to the choice of the metal ion .( )

(ii) For determination of stability constants (βn) in solution, n + 2 independent concentration measurements is needed.( ).

(iii) Among the d^8 systems with similar entering and leaving groups most complexes are comparatively inert.( ).

(iv) In square planar substitution reactions, good entering groups are usually labile leaving groups.( ).

(v) Steric crowding at the center of the reaction inhibits the dissociation reaction.( )

(vi) The π acceptor ligands C_2H_4 and CO greatly accelerates substitution of a ligand that lies trans to itself.

(vii) The rate constant of dissociative intimate mechanism is sensitive to the entering group.( )

(viii) The intimate mechanism for substitution in square planar complexes is energetically associative.( )

(ix) Both associative and dissociative stoichiometric mechanisms are two steps mechanism.( )

(x) Complexes of trivalent f-block metal ions are extremely labile.( )

B) Answer **ONE ONLY** of the following: **(2.5 marks)**

(i) Write three evidence that can justify stoichiometric associative mechanism rather than the intimate one for substitution in $[Pt\,I\,(dien)]^+$ complex. (dien=diethylentriamine).

(ii) Write briefly on the effect of spectator ligand in the substitution of Co (III) or Cr(III) octahedral complexe s.

3- A) Write on **ONE ONLY** of the following: **(8marks)**

(i) Use the trans effect to suggest synthetic routes for preparing cis- and trans $[Pt(NH_3)_4]$ and $[PtCl_4]$.

(ii) Leaving group effect on the hydrolysis of the complex $[CoX(NH_3)_5]^{2+}$

B) Identify organometallic compounds .Which of the following compounds considered to be organometallic and which are not , give reason : **(4.5 marks)**

$(C_3H_7O)_4Ti$, $C_6H_5Ti(OC_3H_7)_3$, CH_3SnCl_3 and CH_3COONa

4- A) Give two ways only of generating metal to carbon bond. **(2 marks)**

B) Prove the multiple nature of the M-CO bond in terms of bond length and vibrational spectra. **(3 marks)**

C) Carbonyl hydrides are slightly soluble in water where they behave as acids, ionizing to give the carbonylate ions. Illustrate that by chemical equations. **(2 marks)**

D) i- From your study of carbon mono-oxide analogs comment on difference between NO and CO as ligands. **(3.5 marks)**

ii- Give the Formals of compounds which are isoelectric with :

$Cr(NO)_4$, $MnCO(NO)_3$, $Ni(CO)_4$ and $Fe(CO)_2(NO)_2$.

E) From your study of alkene complexes give an example to indicate the following facts. **(Answer two points only)** **(2 marks)**

i) Alkene with unconjugated double bonds can form independent linkage to metal atom.

ii) If we have poly olefin involved, the metal atom usually react so as to complete its normal coordination.

iii) Olefin complexes are usually synthesized by interaction of metal carbonyls, halides or other complexes with the olefin.

(Good Luck)

Examiners: 1- Prof .Dr. Said Ahmed Ibrahim
2- Prof. Dr. Sahar Abd Elatif

Assiut University
Faculty of Science
Chemistry Department

(١)

June 2015
Time: 2 hours
(50 Marks)

Second Semester Examination for Geology Group
Subject: Analytical Chemistry (C- 465)

Answer the following questions: **Section(I)**

Q_1) Write on Only Two of the following: **(12.5 Marks)**

a) Describe the absorption phenomena taking place in the far-infrared, near infrared and visible-ultraviolet regions of spectrum.

b) i) Beers law .

ii) A solution containing 1.00 mg of iron (as the thiocyanate complex) in 100ml was observed to absorb 30.0% of the incident light compared to an appropriate blank .

a)What is the absorbance of the solution at this wave length?

b) What fraction of light would be absorbed by a solution of iron four times as concentrated?

c) Give the theoretical bases of spectrophotometric quantification of binary mixtures.

Q_2) Write on Only Two of the following: **(12.5 Marks)**

a) i) Describe the sequence of steps as a sample solution containing analyte A is aspirated into a flame.

ii) Explain how atomic emission result from the hollow cathode lamp.

b) Write briefly on the application of atomic absorption spectroscopy.

c) Atomic fluorescence spectroscopy.

Section(II)

Q_3) Answer Only Two of the following: **(12.5 Marks)**

a) Complete:

i)- In the titration of weak acid with strong base the indicator is -------, while in the titration of weak base with strong acid the indicator is-------.and in the titration of strong acid with strong base the indicators are --------

ii) The half wave potential is------------.

b) Drive the pH for the titration of 100ml 0.1N ammonium hydroxide with **0.1N** HCl at : (k_b= $1.35x10^{-5}$)

i)At the beginning of the titration. - At the end point. - After the end point.

c) Give the reason for the following:

i) Mohr method is applicable in neutral solution.

ii) Supporting electrolyte is used in the polarographic analysis.

Q_4) Answer Only Two of the following: **(12.5 Marks)**

a) Complete:

i) - In Mohr method the indicator is -------- , while in Volhard method -------- or ---------- are used as indicator and in Fajan the indicators are --------------

ii) - The oxidizing agent is ---- and the reducing agent is -------- .

b) Write on the following:

i) The Standard hydrogen electrode.

ii) Applications of potentiometric titration.

ii) Limitation of volumetric precipitation titration reaction.

c) Define Ilkovick equation , then calculate the concentration of lead ions in a solution containing lead gives a diffusion current of 11.7 μA. The diffusion coefficient for lead $1.01x10^{-5}$ cm^2/sec. and the mercury drop characteristics are m = 1.9 mg/sec and t = 3.47 sec/drop.

----------------------------------**Good Luck**-----------------------------

***Examiners**: Prof.Dr. M.A.Ghandour & Prof.Dr .Azza M.M.Ali*

Assiut University
Faculty of Science
Chemistry Department

(11)

Date: June 2015
Time allowed: 3 hours.

Special Topics in Analytical Chemistry Examination (444C)

(Section I) (25 Marks)

<u>I) Answer the following questions:</u> (9 Marks)

1- Describe the equilibrium processes involved in the solvent extraction of metal chelates.

2- Discuss the effect of the pH and of the reagent concentration on the solvent extraction of metal chelates.

II) Answer <u>Four</u> only: (16 Marks)

1- Define or characterize:
i) Solvent extraction ii) Successive extraction

2- Derive a mathematical equation that express the percent extracted.
Define each term used.

3- Ninety percent of a metal chelate is extracted when equal volumes of aqueous and organic phases are used. What will be the percent extracted if the volume of the organic phase is doubled?

4- For the extraction of benzoic acid:
i) Write the relation between D & K_D, Define each term used.
ii) Discuss the effect of the pH on this relation.

5- Ninety-six percent of a solute is removed from 100 ml of an aqueous solution by extraction with two 50-ml portions of an organic solvent. What is the distribution coefficient of the solute?

Section (II) (25 Marks)

<u>Answer the following questions :</u>

<u>First Question :</u> **(9 Marks)**

1- Describe a spectrophotometric method (involving the mechanism) for the determination of dopamine drug through the complexation of dopa-semiquinone with Ni(ii) ions.

2- Explain the energy scheme of various types of electron excitations for Ultraviolet/Visible spectra of organic molecules.

3- Define each of the following terms: Accuracy - Limit of quantitation - Selectivity - Ruggedness.

<u>أنظر خلفه باقي الاسئلة.</u>

(2)

Second Question: Answer Four only of the following: **(16 Marks)**

1- Illustrate the scheme proposed for secnidazole drug reacting with sodium nitrite in the presence of hydrochloric acid. Describe the reaction involving the mechanism between diazotized drug and 2,5-Dihydroxy benzoic acid as a coupling agent to form the azo product.

2- How can you validate the spectrophotometric measurements of a pharmaceutical substance.

3- Describe a spectrophotometric method (involving the mechanism) for the determination of norepinephrine drug by oxidation with sodium iodate.

4- Suggest a spectrophotometric method for the detection of Fluoroquinolone antibacterial (Norfloxacin) drug by forming binary complex between the drug and Eosin Y dye.

5- Describe the scheme proposed for indirect determination of ascorbic acid by oxidation with $HgCl_2$ and reaction of oxidation product with 4,5-dimethyl-o-phenylendiamine.

" Good Luck "

Examiners : Prof. Dr. Hassan Sedaira
Dr. Ahmed Mohamed Kamal

(1)

Chemistry Department,
Faculty of Science,
Assiut University

June 2015

Time: 3 Hours

Final Exam In Selected Topics in Organic Chemistry (Chem.414)

Answer the following questions: **Marks: 50**

Section A(Supramolecular Organic Chemistry) **Marks: 16**

1-Classify Supramolecular Host- Guest Compounds (2 Marks)

2-What are Recptors and discuss the Lock-Key Principle (3 Marks)

3-Define Preorganization and Complementarity (3 Marks)

4-What are the different categories of Supramolecular interactions (8 Marks)

Section B: **Marks: 17**

Answer the following questions:

1- (i) Give an account on the following terms: (8 Marks)

(a) The differences between nucleotides and nucleosides with examples.

(b) Mutation and its types.

(c) The function of mRNA.

(d) The structure of nucleic acids (RNA and DNA).

(ii) The following section of DNA is used to build mRNA for a protein:

T A C-T C G-G A G **(3 Marks)**

(a) What is the corresponding mRNA sequence?

(b) What is the amino acid order in the peptide?

(c) What are the anticodons on the tRNAs?

2- (i) Draw the structures of the following species: (4 Marks)

(a) Adenosine.

(b) Adenosine 5'-monophosphate (AMP).

(c) Deoxyguanosine.

(d) Azidothymine (AZT).

(c)

(e) Deoxycytidine 5'-monophosphate (dCMP).

(ii) Give short notes on the steps of protein synthesis. **(2 Marks)**

Section C: Biochemistry:

Answer three (3) of the following: **(17 Marks)**

(a) Write on two only of the cases in which sugar appears in urine.

(b) Write on the reactions involved in uronic acid pathway and its biological importance.

(c) Scheme out the reactions involved in B-oxidation of a fatty acid containing 6 carbon atoms .Calculate the energy stored in ATP molecules during this process.

(d) Show by equations how acetylcoenzymeAis transformed into mevalonic acid.

Good Luck

Prof. Dr. A. T. Hamam

Prof. Dr. A. M. Elkhawaga

Dr. A. A. Omer

(1)

Chemistry Department
Faculty of Science
Assiut University

June, 2015
Time: 2 hours
50 Marks

Final Exam of Petroleum & Petrochemicals (451C) for the 3rd Petroleum Geology Level Students

Answer the following questions:

1- I- Answer *two* only of the following: (10 Marks)

a) Describe in details the thermal conversion processes (Visbreaking & Delayed coking)?
b) Oxygen compounds as petroleum compositions.
c) Outline the importance petrochemicals based on methane?.

II- Draw and discuss of thermoform catalytic cracking process.

2- I- Explain briefly *two* only of the following: (10 Marks)

a) Doctor's sweetening process equations.
b) Advantages and disadvantages of catalytic cracking.
c) Isomerization mechanism (*n*-Alkanes into isoparaffins).

II- Draw and discuss of vacuum distillation process for the residual products.

3- I- write a short notes of *two* only of the following: (10 Marks)

a) Asphaltic-Base crude oils.
b) Describe the basic processes encountered in the petroleum refining operations?
c) Discuss the effect of sulphur compounds on petroleum products?

II- Draw and discuss chemical and electric desalting processes.

4- I- Give an account *two* only on the following: (10 Marks)

a) Viscosity index and its examples.
b) Explain in detail the polymerization reactions of light olefin gases?
c) Diesel index and its importance.

II- Outline the hydrocracking and hydrodealkylation reactions of heavy oils over zeolite catalyst?

5- I- Discuss *two* only of the following points: (10 Marks)

a) Smoke point and its uses.
b) Carbide theory is one of the origin of petroleum crudes in nature.
c) Octane number and all its additives.

II- Detail the purpose and merits of hydrocraking process of heavier feedstock.

Good Luck

Prof. Dr. Abdel-Aal Gaber
Dr. Hassan A. Kotb

Assiut University

Surface Chemistry & Electrochemistry for 4th Level students (Chem.434)

(Chemistry Major)

(١)

Faculty of Science
Chemistry Department

Time: 3 hrs.
Date : Jun. 2015

Answer the Following Questions:

Section (I) Surface Chemistry

1. Answer the following question:

1. Define the following terms: **(6 Marks)**

i) Chemisorption ii) Specifity of the adsorption iii) Heterogeneous catalysis
iv) Turnover number iv) Active sites v) Sintering process.

2. Write short notes on three only of the following: **(12 Marks)**

a) Factors affecting the surface area of a solid powder.
b) Non- stoichiometry of solid compounds.
c) Dislocations in solids.
d) Role of the catalyst during the chemical reactions.

3. Answer three only of the following: **(15 Marks)**

(a) What are the desired properties of a support and why alumina is the most important one.
(b) Apply the V_{a-t} plot for determination of S_t and the porosity of the catalyst.
(c) Discuss the effect of lower and higher valences on the electrical conductivity of NiO.
(d) Explain the role of promoters on the physiochemical properties of a catalyst.

Section (2) Electrochemistry

Answer the following:

1) a) For silver-silver ion electrode reaction: $Ag^{+}_{(aq)} + e^- = Ag_{(s)}$

$$\text{The rate} = k_{chem,f}\, C_{Ag+}\, e^{\frac{-\beta F\Delta\phi}{RT}} - k_{chem,b}\, e^{\frac{(1-\beta)F\Delta\phi}{RT}}$$

Define the parameters, $k_{chem,f}$, $k_{chem,b}$, C_{Ag+}, β, and $\Delta\varphi$, and starting from this equation drive the Butler-Volmer equation. **(5marks)**

b) Using Tafel equation calculate the exchange current (I_o) for reduction of ferric ion (Fe^{3+}) to ferrous ion (Fe^{2+}) on platinum electrode (1 cm^2) by applying 0.65 V and the resulted current is 0.0122 A where E_o = 0.75 V, β = 0.46, R = 8.314 JK-1mol-1, F = 96485 C and T= 293 K.

(5marks)

2) **Answer only one from the following**

I) a) Starting with the first law of thermodynamic (dU=dq+dw) indicate that the measurement of a cell potential directly calculates the Gibbs free energy change for the process. **(4marks)**

b) What is the ionic strength of an electrolyte contains 0.25 M $Al(NO_3)_3$. **(3marks)**

II) a) Write on: Galvani potential difference and its composition – Cathodic protection. **(4marks)**

b) Write three limitations of the Debye – Huckel Limiting Law. **(3marks)**

Good Luck

Prof. Abd El-Aziz A. Said
Prof. Abo-Elhagag A. Mohamed

Assiut University

Faculty of Science
Chemistry Department

Final Examination for B.Sc. (Chemistry major)
Applied Organic Chemistry (412 C): (Textiles& Dyes & Polymers &Material science)

Date: Sunday, 07/06/2015 Time: 2 hours.

Answer the following Two Sections:

Section A: (Textiles and Dyes Chemistry). **(25 points)**

Answer the following:

1) Physical properties of fibers determine its endues:
   Locate and discuss the following :
   a. Resiliency. b. Crimps c. Absorbancy d. Wool in burning test.
2) Tabulate the morphology and chemical structure of cotton and wool fibers.
3) Answer **one** of the following :
   a) Chemical Reactions of Cotton related to industry.
   b) Treatment of Cotton before dyeing.

Section B : (Polymers &Material Science) **(25 Points)**

Answer the following questions:

1) a) " Carbon Fibers........ the wonder polymer......... stronger than the steel".
   Show by equations the steps of production of this polymer.
   b) Show the mechanism of opening the caprolactam ring to form Nylon 6.
2) a) Discuss with examples the types of Initiators.
   b) The presence of alkyl group in propylene monomer fail it to polymerized. Discuss.
3) a) $Al(CH_3)_3 + TiCl_4 + CH_2=CH_2 \rightarrow$
   Show the mechanism of its coordination polymerization.
   b) Discuss how the polyurethane combine both the addition and condensation polymerization.
4) a) Is it possible to make polyethylene from cyclohexane? If not, say why?
   b) In the living polymerization, show by equations how can we put an ending for the living chain. (Carbanion).

Good Luck

Examiners:

Prof. Dr. Saud A Metwally& Prof. Dr. Kamal I Aly

(1)

Assiut University
Faculty of Science
Chemistry Department

Time allowed: three hours

Final Exam for Course No-423 (May 2015)

Answer the following question: **(10 Marks)**

a) For the following space groups

P4/m, F222, Pmna, P4/n, R3m, P6mm, P2/m3¯, P32,P6mm

Define the crystal system, crystal class and Laue symmetry.

b) Describe in details the full symmetry elements in *P2/m3¯* space group.

Answer Four only of the following questions:

(10 Marks)

1- a) Describe in details the structure of rock salt , zinc blende and antifluorite structures in terms of close packing and space filling polyhedral approaches.

1- b) Starting from a rock salt structure, what structures are generated by the following imaginary steps.

i) Removal of all atoms or ions of one type.

ii) Removal of alternate layers of cations.

iii) Replacement of all cations in O sites by an equal number of cations in T+ sites.

1- c) Calculate the d and 2θ values for the 111 line in XRD Cu kα radiation(λ= 1.54A°) of a cubic substance with a = 5.0 A°

1- d) What is the probable lattice type of crystalline substances that give the following observed reflections

110, 200, 103, 202, 211
111, 200, 113, 220, 222
100, 110, 111, 200, 210
001, 110, 200, 111, 201

(10 Marks)

2- a) X-ray of an unknown wave length are diffracted by a gold sample. The 2θ angle was 64.58° for the [220] plane. What is the wave length of the X-ray used.
(the lattice constant of gold = 4.0788A°).

2- b) $LiSrH_3$ crystallize as a white cubic solid after the reaction of Li and Sr under a flow of hydrogen at 600C°.

What factors affect the scattering of x-ray by crystalline solids. Why might this compound be difficult to characterize.

The powder x-ray diffraction pattern of this material show the following reflections

2θ = 23.25 , 40.84 ,47.53 ,53.56 ,69.49 and 74.38°.

Index the data , determine the lattice type and calculate the cell parameter (λ = 1.54 A°)

(5)

(10 Marks)

3- Debye- Sherrer pattern of tungsten (BCC) is made with CuKα radiation (λ= 1.54A°). The first four lines on this pattern were observed to have the following 2 Θ values

line	θ°
1	20.3
2	29.2
3	36.7
4	43.6

i) Index these lines

ii) Calculate the intensity of the first line

(10 Marks)

4- For CsCl crystal

i) What are the fraction coordinates of these two atoms.

ii) Derive a simplified structure factor equation for this. Can you observe the lines 100.

(10 Marks)

5- a) Derive simplified expression for F^2 for ZnS blende (FCC), including the rules governing the observed reflections. Calculate the relative intensity of the line 444.

5- b) What are the basic symmetry elements in the following crystal systems.

Trigonal, hexagonal, monoclinic, Orthorhombic.

Good Luck

Prof.Dr.R.M.Mahfouz

1

APPENDIX 11

VALUES OF $(\sin\theta)/\lambda$ (Å^{-1})

θ	Radiation				
	Mo $K\alpha$ (0.711 Å)	Cu $K\alpha$ (1.542 Å)	Co $K\alpha$ (1.790 Å)	Fe $K\alpha$ (1.937 Å)	Cr $K\alpha$ (2.291 Å)
0°	0.00	0.00	0.00	0.00	0.00
1	0.02	0.01	0.01	0.01	0.01
2	0.05	0.02	0.02	0.02	0.02
3	0.07	0.03	0.03	0.03	0.02
4	0.10	0.05	0.04	0.04	0.03
5	0.12	0.06	0.05	0.04	0.04
6	0.15	0.07	0.06	0.05	0.05
7	0.17	0.08	0.07	0.06	0.05
8	0.20	0.09	0.08	0.07	0.06
9	0.22	0.10	0.09	0.08	0.07
10	0.24	0.11	0.10	0.09	0.08
11	0.27	0.12	0.11	0.10	0.08
12	0.29	0.13	0.12	0.11	0.09
13	0.32	0.15	0.13	0.12	0.10
14	0.34	0.16	0.14	0.12	0.11
15	0.36	0.17	0.14	0.13	0.11
16	0.39	0.18	0.15	0.14	0.12
17	0.41	0.19	0.16	0.15	0.13
18	0.43	0.20	0.17	0.16	0.13
19	0.46	0.21	0.18	0.17	0.14
20	0.48	0.22	0.19	0.18	0.15
21	0.51	0.23	0.20	0.18	0.15
22	0.53	0.24	0.21	0.19	0.16
23	0.55	0.25	0.22	0.20	0.17
24	0.57	0.26	0.23	0.21	0.18
25	0.60	0.27	0.24	0.22	0.18
26	0.62	0.28	0.24	0.23	0.19
27	0.64	0.29	0.25	0.23	0.20
28	0.66	0.30	0.26	0.24	0.20
29	0.68	0.31	0.27	0.25	0.21

2)

	Radiation				
	Mo $K\alpha$ (0.711 Å)	Cu $K\alpha$ (1.542 Å)	Co $K\alpha$ (1.790 Å)	Fe $K\alpha$ (1.937 Å)	Cr $K\alpha$ (2.291 Å)
30	0.70	0.32	0.28	0.26	0.22
31	0.72	0.33	0.29	0.27	0.22
32	0.75	0.34	0.30	0.27	0.23
33	0.77	0.35	0.30	0.28	0.24
34	0.79	0.36	0.31	0.29	0.24
35	0.81	0.37	0.32	0.29	0.25
36	0.83	0.38	0.33	0.30	0.26
37	0.85	0.39	0.34	0.31	0.26
38	0.87	0.40	0.34	0.32	0.27
39	0.89	0.41	0.35	0.32	0.27
40	0.91	0.42	0.36	0.33	0.28
41	0.93	0.43	0.37	0.34	0.29
42	0.94	0.43	0.37	0.35	0.29
43	0.96	0.44	0.38	0.35	0.30
44	0.98	0.45	0.39	0.36	0.30
45	0.99	0.46	0.40	0.36	0.31
46	1.01	0.47	0.40	0.37	0.31
47	1.03	0.47	0.41	0.38	0.32
48	1.05	0.48	0.42	0.38	0.32
49	1.06	0.49	0.42	0.39	0.33
50	1.08	0.50	0.43	0.39	0.33
52	1.11	0.51	0.44	0.41	0.34
54	1.14	0.52	0.45	0.42	0.35
56	1.17	0.54	0.46	0.43	0.36
58	1.20	0.55	0.47	0.44	0.37
60	1.22	0.56	0.48	0.45	0.38
62	1.24	0.57	0.49	0.46	0.39
64	1.26	0.58	0.50	0.46	0.39
66	1.28	0.59	0.51	0.47	0.40
68	1.30	0.60	0.52	0.48	0.40
70	1.32	0.61	0.53	0.48	0.41
72	1.34	0.62	0.53	0.49	0.41
74	1.35	0.62	0.54	0.50	0.42
76	1.37	0.63	0.54	0.50	0.42
78	1.38	0.63	0.55	0.50	0.43
80	1.39	0.64	0.55	0.51	0.43
82	1.39	0.64	0.55	0.51	0.43
84	1.40	0.64	0.56	0.51	0.43
86	1.40	0.65	0.56	0.51	0.43
88	1.41	0.65	0.56	0.52	0.43
90	1.41	0.65	0.56	0.52	0.43

3

$\frac{\sin\theta}{\lambda}$ (Å^{-1})	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0		
H	1	0.81	0.48	0.25	0.13	0.07	0.04	0.03	0.02	0.01	0.00	[illegible]	
He	2	1.88	1.46	1.05	0.75	0.52	0.35	0.24	0.18	0.14	0.11	[illegible]	
Li^{+}	2	1.96	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4	0.3	0.3	
Li	3	2.2	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4	0.3	0.3	
Be^{+2}	2	2.0	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7	0.6	0.5	
Be	4	2.9	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7	0.6	0.5	
B^{+3}	2	1.99	1.9	1.8	1.7	1.6	1.4	1.3	1.2	1.0	0.9	0.7	
B	5	3.5	2.4	1.9	1.7	1.5	1.4	1.2	1.2	1.0	0.9	0.7	
C	6	4.6	3.0	2.2	1.9	1.7	1.6	1.4	1.3	1.16	1.0	0.9	
N^{+5}	2	2.0	2.0	1.9	1.9	1.8	1.7	1.6	1.5	1.4	1.3	1.16	
N^{+3}	4	3.7	3.0	2.4	2.0	1.8	1.66	1.56	1.49	1.39	1.28	1.17	
N	7	5.8	4.2	3.0	2.3	1.9	1.65	1.54	1.49	1.39	1.29	1.17	
O	8	7.1	5.3	3.9	2.9	2.2	1.8	1.6	1.5	1.4	1.35	1.26	
O^{-2}	10	8.0	5.5	3.8	2.7	2.1	1.8	1.5	1.5	1.4	1.35	1.26	
F	9	7.8	6.2	4.45	3.35	2.65	2.15	1.9	1.7	1.6	1.5	1.35	
F^{-}	10	8.7	6.7	4.8	3.5	2.8	2.2	1.9	1.7	1.55	1.5	1.35	
Ne	10	9.3	7.5	5.8	4.4	3.4	2.65	2.2	1.9	1.65	1.55	1.5	
Na^{+}	10	9.5	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95	1.75	1.6	
Na	11	9.65	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95	1.75	1.6	
Mg^{+2}	10	9.75	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2	2.0	1.8	
Mg	12	10.5	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2	2.0	1.8	
Al^{+3}	10	9.7	8.9	7.8	6.65	5.5	4.45	3.65	3.1	2.65	2.3	2.0	
Al	13	11.0	8.95	7.75	6.6	5.5	4.5	3.7	3.1	2.65	2.3	2.0	
Si^{+4}	10	9.75	9.15	8.25	7.15	6.05	5.05	4.2	3.4	2.95	2.6	2.3	
Si	14	11.35	9.4	8.2	7.15	6.1	5.1	4.2	3.4	2.95	2.6	2.3	
P^{+5}	10	9.8	9.25	8.45	7.5	6.55	5.65	4.8	4.05	3.4	3.0	2.6	
P	15	12.4	10.0	8.45	7.45	6.5	5.65	4.8	4.05	3.4	3.0	2.6	
P^{-3}	18	12.7	9.8	8.4	7.45	6.5	5.65	4.85	4.05	3.4	3.0	2.6	
S^{+6}	10	9.85	9.4	8.7	7.85	6.85	6.05	5.25	4.5	3.9	3.35	2.9	
S	16	13.6	10.7	8.95	7.85	6.85	6.0	5.25	4.5	3.9	3.35	2.9	
S^{-2}	18	14.3	10.7	8.9	7.85	6.85	6.0	5.25	4.5	3.9	3.35	2.9	
Cl	17	14.6	11.3	9.25	8.05	7.25	6.5	5.75	5.05	4.4	3.85	3.35	
Cl^{-}	18	15.2	11.5	9.3	8.05	7.25	6.5	5.75	5.05	4.4	3.85	3.35	
A	18	15.9	12.6	10.4	8.7	7.8	7.0	6.2	5.4	4.7	4.1	3.6	
K^{+}	18	16.5	13.3	10.8	8.85	7.75	7.05	6.44	5.9	5.3	4.8	4.2	
K	19	16.5	13.3	10.8	9.2	7.9	6.7	5.9	5.2	4.6	4.2	3.7	3.3
Ca^{+2}	18	16.8	14.0	11.5	9.3	8.1	7.35	6.7	6.2	5.7	5.1	4.6	
Ca	20	17.5	14.1	11.4	9.7	8.4	7.3	6.3	5.6	4.9	4.5	4.0	3.6
Sc^{+3}	18	16.7	14.0	11.4	9.4	8.3	7.6	6.9	6.4	5.8	5.35	4.85	
Sc	21	18.4	14.9	12.1	10.3	8.9	7.7	6.7	5.9	5.3	4.7	4.3	3.9
Ti^{+4}	18	17.0	14.4	11.9	9.9	8.5	7.85	7.3	6.7	6.15	5.65	5.05	
Ti	22	19.3	15.7	12.8	10.9	9.5	8.2	7.2	6.3	5.6	5.0	4.6	4.2
V	23	20.2	16.6	13.5	11.5	10.1	8.7	7.6	6.7	5.9	5.3	4.9	4.4
Cr	24	21.1	17.4	14.2	12.1	10.6	9.2	8.0	7.1	6.3	5.7	5.1	4.6
Mn	25	22.1	18.2	14.9	12.7	11.1	9.7	8.4	7.5	6.6	6.0	5.4	4.9

(4)

		0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2
		26	23.1	18.9	15.6	13.3	11.6	10.2	8.9	7.9	7.0	6.3	5.7	5.2
Co		27	24.1	19.8	16.4	14.0	12.1	10.7	9.3	8.3	7.3	6.7	6.0	5.5
Ni		28	25.0	20.7	17.2	14.6	12.7	11.2	9.8	8.7	7.7	7.0	6.3	5.8
Cu		29	25.9	21.6	17.9	15.2	13.3	11.7	10.2	9.1	8.1	7.3	6.6	6.0
Zn		30	26.8	22.4	18.6	15.8	13.9	12.2	10.7	9.6	8.5	7.6	6.9	6.3
Ga		31	27.8	23.3	19.3	16.5	14.5	12.7	11.2	10.0	8.9	7.9	7.3	6.7
Ge		32	28.8	24.1	20.0	17.1	15.0	13.2	11.6	10.4	9.3	8.3	7.6	7.0
As		33	29.7	25.0	20.8	17.7	15.6	13.8	12.1	10.8	9.7	8.7	7.9	7.3
Se		34	30.6	25.8	21.5	18.3	16.1	14.3	12.6	11.2	10.0	9.0	8.2	7.5
Br		35	31.6	26.6	22.3	18.9	16.7	14.8	13.1	11.7	10.4	9.4	8.6	7.8
Kr		36	32.5	27.4	23.0	19.5	17.3	15.3	13.6	12.1	10.8	9.8	8.9	8.1
Rb^+		36	33.6	28.7	24.6	21.4	18.9	16.7	14.6	12.8	11.2	9.9	8.9	
Rb		37	33.5	28.2	23.8	20.2	17.9	15.9	14.1	12.5	11.2	10.2	9.2	8.4
Sr		38	34.4	29.0	24.5	20.8	18.4	16.4	14.6	12.9	11.6	10.5	9.5	8.7
Y		39	35.4	29.9	25.3	21.5	19.0	17.0	15.1	13.4	12.0	10.9	9.9	9.0
Zr		40	36.3	30.8	26.0	22.1	19.7	17.5	15.6	13.8	12.4	11.2	10.2	9.3
Nb		41	37.3	31.7	26.8	22.8	20.2	18.1	16.0	14.3	12.8	11.6	10.6	9.7
Mo		42	38.2	32.6	27.6	23.5	20.8	18.6	16.5	14.8	13.2	12.0	10.9	10.0
Tc		43	39.1	33.4	28.3	24.1	21.3	19.1	17.0	15.2	13.6	12.3	11.3	10.3
Ru		44	40.0	34.3	29.1	24.7	21.9	19.6	17.5	15.6	14.1	12.7	11.6	10.6
Rh		45	41.0	35.1	29.9	25.4	22.5	20.2	18.0	16.1	14.5	13.1	12.0	11.0
Pd		46	41.9	36.0	30.7	26.2	23.1	20.8	18.5	16.6	14.9	13.6	12.3	11.3
Ag		47	42.8	36.9	31.5	26.9	23.8	21.3	19.0	17.1	15.3	14.0	12.7	11.7
Cd		48	43.7	37.7	32.2	27.5	24.4	21.8	19.6	17.6	15.7	14.3	13.0	12.0
In		49	44.7	38.6	33.0	28.1	25.0	22.4	20.1	18.0	16.2	14.7	13.4	12.3
Sn		50	45.7	39.5	33.8	28.7	25.6	22.9	20.6	18.5	16.6	15.1	13.7	12.7
Sb		51	46.7	40.4	34.6	29.5	26.3	23.5	21.1	19.0	17.0	15.5	14.1	13.0
Te		52	47.7	41.3	35.4	30.3	26.9	24.0	21.7	19.5	17.5	16.0	14.5	13.3
I		53	48.6	42.1	36.1	31.0	27.5	24.6	22.2	20.0	17.9	16.4	14.8	13.6
Xe		54	49.6	43.0	36.8	31.6	28.0	25.2	22.7	20.4	18.4	16.7	15.2	13.9
Cs		55	50.7	43.8	37.6	32.4	28.7	25.8	23.2	20.8	18.8	17.0	15.6	14.5
Ba		56	51.7	44.7	38.4	33.1	29.3	26.4	23.7	21.3	19.2	17.4	16.0	14.7
La		57	52.6	45.6	39.3	33.8	29.8	26.9	24.3	21.9	19.7	17.9	16.4	15.0
Ce		58	53.6	46.5	40.1	34.5	30.4	27.4	24.8	22.4	20.2	18.4	16.6	15.3
Pr		59	54.5	47.4	40.9	35.2	31.1	28.0	25.4	22.9	20.6	18.8	17.1	15.7
Nd		60	55.4	48.3	41.6	35.9	31.8	28.6	25.9	23.4	21.1	19.2	17.5	16.1
Pm		61	56.4	49.1	42.4	36.6	32.4	29.2	26.4	23.9	21.5	19.6	17.9	16.4
Sm		62	57.3	50.0	43.2	37.3	32.9	29.8	26.9	24.4	22.0	20.0	18.3	16.8
Eu		63	58.3	50.9	44.0	38.1	33.5	30.4	27.5	24.9	22.4	20.4	18.7	17.1
Gd		64	59.3	51.7	44.8	38.8	34.1	31.0	28.1	25.4	22.9	20.8	19.1	17.5
Tb		65	60.2	52.6	45.7	39.6	34.7	31.6	28.6	25.9	23.4	21.2	19.5	17.9
Dy		66	61.1	53.6	46.5	40.4	35.4	32.2	29.2	26.3	23.9	21.6	19.9	18.3
Ho		67	62.1	54.5	47.3	41.1	36.1	32.7	29.7	26.8	24.3	22.0	20.3	18.6
Er		68	63.0	55.3	48.1	41.7	36.7	33.3	30.2	27.3	24.7	22.4	20.7	18.9
Tm		69	64.0	56.2	48.9	42.4	37.4	33.9	30.8	27.9	25.2	22.9	21.0	19.3

5

$\frac{\sin\theta}{\lambda}$ (Å^{-1})	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2
Yb	70	64.9	57.0	49.7	43.2	38.0	34.4	31.3	28.4	25.7	23.3	21.4	19.7
Lu	71	65.9	57.8	50.4	43.9	38.7	35.0	31.8	28.9	26.2	23.8	21.8	20.0
Hf	72	66.8	58.6	51.2	44.5	39.3	35.6	32.3	29.3	26.7	24.2	22.3	20.4
Ta	73	67.8	59.5	52.0	45.3	39.9	36.2	32.9	29.8	27.1	24.7	22.6	20.9
W	74	68.8	60.4	52.8	46.1	40.5	36.8	33.5	30.4	27.6	25.2	23.0	21.3
Re	75	69.8	61.3	53.6	46.8	41.1	37.4	34.0	30.9	28.1	25.6	23.4	21.6
Os	76	70.8	62.2	54.4	47.5	41.7	38.0	34.6	31.4	28.6	26.0	23.9	22.0
Ir	77	71.7	63.1	55.3	48.2	42.4	38.6	35.1	32.0	29.0	26.5	24.3	22.3
Pt	78	72.6	[illegible]	56.2	48.9	43.1	39.2	35.6	32.5	29.5	27.0	24.7	22.7
Au	79	73.6	[illegible]	57.0	49.7	43.8	39.8	36.2	33.1	30.0	27.4	25.1	23.1
Hg	80	74.6	65.9	57.9	50.5	44.4	40.5	36.8	33.6	30.6	27.8	25.6	23.6
Tl	81	75.5	66.7	58.7	51.2	45.0	41.1	37.4	34.1	31.1	28.3	26.0	24.1
Pb	82	76.5	67.5	59.5	51.9	45.7	41.6	37.9	34.6	31.5	28.8	26.4	24.5
Bi	83	77.5	68.4	60.4	52.7	46.4	42.2	38.5	35.1	32.0	29.2	26.8	24.8
Po	84	78.4	69.4	61.3	53.5	47.1	42.8	39.1	35.6	32.6	29.7	27.2	25.2
At	85	79.4	70.3	62.1	54.2	47.7	43.4	39.6	36.2	33.1	30.1	27.6	25.6
Rn	86	80.3	71.3	63.0	55.1	48.4	44.0	40.2	36.8	33.5	30.5	28.0	26.0
Fr	87	81.3	72.2	63.8	55.8	49.1	44.5	40.7	37.3	34.0	31.0	28.4	26.4
Ra	88	82.2	73.2	64.6	56.5	49.8	45.1	41.3	37.8	34.6	31.5	28.8	26.7
Ac	89	83.2	74.1	65.5	57.3	50.4	45.8	41.8	38.3	35.1	32.0	29.2	27.1
Th	90	84.1	75.1	66.3	58.1	51.1	46.5	42.4	38.8	35.5	32.4	29.6	27.5
Pa	91	85.1	76.0	67.1	58.8	51.7	47.1	43.0	39.3	36.0	32.8	30.1	27.9
U	92	86.0	76.9	67.9	59.6	52.4	47.7	43.5	39.8	36.5	33.3	30.6	28.3
Np	93	87	78	69	60	53	48	44	40	37	34	31	29
Pu	94	88	79	69	61	54	49	44	41	38	34	31	29
Am	95	89	79	70	62	55	50	45	42	38	35	32	30
Cm	96	90	80	71	62	55	50	46	42	39	35	32	30
Bk	97	91	81	72	63	56	51	46	43	39	36	33	30
Cf	98	92	82	73	64	57	52	47	43	40	36	33	31
	99	93	83	74	65	57	52	48	44	40	37	34	31
	100	94	84	75	66	58	53	48	44	41	37	34	31

From Peiser, Rooksby, and Wilson [G.13]. More extensive tables, at smaller intervals of $(\sin\theta)/\lambda$, are given on pp. 72–98 of Vol. 4 of [G.11].

6

APPENDIX 13
MULTIPLICITY FACTORS FOR THE POWDER METHOD

					111		
Cubic:	*hkl*	*hhl*	0*kl*	0*kk*	*hhh*	00*l*	
	48*	24	24*	12	8	6	
Hexagonal and Rhombohedral:	*hk* · *l*	*hh* · *l*	0*k* · *l*	*hk* · 0	*hh* · 0	0*k* · 0	00 · *l*
	24*	12*	12*	12*	6	6	2
Tetragonal:	*hkl*	*hhl*	0*kl*	*hk*0	*hh*0	0*k*0	00*l*
	16*	8	8	8*	4	4	2
Orthorhombic:	*hkl*	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*
	8	4	4	4	2	2	2
Monoclinic:	*hkl*	*h*0*l*	0*k*0				
	4	2	2				
Triclinic:	*hkl*						
	2						

Note that, in cubic crystals, for example, *hhl* stands for such indices as 112 (or 211), 0*kl* for such indices as 012 (or 210), 0*kk* for such indices as 011 (or 110), etc.

* These are the usual multiplicity factors. In some crystals, planes having these indices comprise two forms with the same spacing but different structure factor, and the multiplicity factor for each form is half the value given above. In the cubic system, for example, there are some crystals in which permutations of the indices (*hkl*) produce planes which are not structurally equivalent; in such crystals (AuBe, discussed in Sec. 2–7, is an example), the plane (123), for example, belongs to one form and has a certain structure factor, while the plane (321) belongs to another form and has a different structure factor. There are $\frac{48}{2} = 24$ planes in the first form and 24 planes in the second. This question is discussed more fully by Henry, Lipson, and Wooster [G.8].

APPENDIX 14

LORENTZ-POLARIZATION FACTOR $\left(\dfrac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}\right)$

7

$\theta°$	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9
2	1639	1486	1354	1239	1138	1048	968.9	898.3	835.1	778.4
3	727.2	680.9	638.8	600.5	565.6	533.6	504.3	477.3	452.3	429.3
4	408.0	388.2	369.9	352.7	336.8	321.9	308.0	294.9	282.6	271.1
5	260.3	250.1	240.5	231.4	222.9	214.7	207.1	199.8	192.9	186.3
6	180.1	174.2	168.5	163.1	158.0	153.1	148.4	144.0	139.7	135.6
7	131.7	128.0	124.4	120.9	117.6	114.4	111.4	108.5	105.6	102.9
8	100.3	97.80	95.37	93.03	90.78	88.60	86.51	84.48	82.52	80.63
9	78.79	77.02	75.31	73.66	72.05	70.49	68.99	67.53	66.12	64.74
10	63.41	62.12	60.87	59.65	58.46	57.32	56.20	55.11	54.06	53.03
11	52.04	51.06	50.12	49.19	48.30	47.43	46.58	45.75	44.94	44.16
12	43.39	42.64	41.91	41.20	40.50	39.82	39.16	38.51	37.88	37.27
13	36.67	36.08	35.50	34.94	34.39	33.85	33.33	32.81	32.31	31.82
14	31.34	30.87	30.41	29.96	29.51	29.08	28.66	28.24	27.83	27.44
15	27.05	26.66	26.29	25.92	25.56	25.21	24.86	24.52	24.19	23.86
16	23.54	23.23	22.92	22.61	22.32	22.02	21.74	21.46	21.18	20.91
17	20.64	20.38	20.12	19.87	19.62	19.38	19.14	18.90	18.67	18.44
18	18.22	18.00	17.78	17.57	17.36	17.15	16.95	16.75	16.56	16.36
19	16.17	15.99	15.80	15.62	15.45	15.27	15.10	14.93	14.76	14.60
20	14.44	14.28	14.12	13.97	13.81	13.66	13.52	13.37	13.23	13.09
21	12.95	12.81	12.68	12.54	12.41	12.28	12.15	12.03	11.91	11.78
22	11.66	11.54	11.43	11.31	11.20	11.09	10.98	10.87	10.76	10.65
23	10.55	10.45	10.35	10.24	10.15	10.05	9.951	9.857	9.763	9.671
24	9.579	9.489	9.400	9.313	9.226	9.141	9.057	8.973	8.891	8.810
25	8.730	8.651	8.573	8.496	8.420	8.345	8.271	8.198	8.126	8.054
26	7.984	7.915	7.846	7.778	7.711	7.645	7.580	7.515	7.452	7.389
27	7.327	7.266	7.205	7.145	7.086	7.027	6.969	6.912	6.856	6.800
28	6.745	6.692	6.637	6.584	6.532	6.480	6.429	6.379	6.329	6.279
29	6.230	6.183	6.135	6.088	6.042	5.995	5.950	5.905	5.861	5.817
30	5.774	5.731	5.688	5.647	5.605	5.564	5.524	5.484	5.445	5.406
31	5.367	5.329	5.292	5.254	5.218	5.181	5.145	5.110	5.075	5.040
32	5.006	4.972	4.939	4.906	4.873	4.841	4.809	4.777	4.746	4.715
33	4.685	4.655	4.625	4.595	4.566	4.538	4.509	4.481	4.453	4.426
34	4.399	4.372	4.346	4.320	4.294	4.268	4.243	4.218	4.193	4.169
35	4.145	4.121	4.097	4.074	4.052	4.029	4.006	3.984	3.962	3.941
36	3.919	3.898	3.877	3.857	3.836	3.816	3.797	3.777	3.758	3.739
37	3.720	3.701	3.683	3.665	3.647	3.629	3.612	3.594	3.577	3.561
38	3.544	3.527	3.513	3.497	3.481	3.465	3.449	3.434	3.419	3.404
39	3.389	3.375	3.361	3.347	3.333	3.320	3.306	3.293	3.280	3.268
40	3.255	3.242	3.230	3.218	3.206	3.194	3.183	3.171	3.160	3.149
41	3.138	3.127	3.117	3.106	3.096	3.086	3.076	3.067	3.057	3.048
42	3.038	3.029	3.020	3.012	3.003	2.994	2.986	2.978	2.970	2.962
43	2.954	2.946	2.939	2.932	2.925	2.918	2.911	2.904	2.897	2.891
44	2.884	2.878	2.872	2.866	2.860	2.855	2.849	2.844	2.838	2.833

8

θ°	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9
45	2.828	2.824	2.819	2.814	2.810	2.805	2.801	2.797	2.793	2.789
46	2.785	2.782	2.778	2.775	2.772	2.769	2.766	2.763	2.760	2.757
47	2.755	2.752	2.750	2.748	2.746	2.744	2.742	2.740	2.738	2.737
48	2.736	2.735	2.733	2.732	2.731	2.730	2.730	2.729	2.729	2.728
49	2.728	2.728	2.728	2.728	2.728	2.728	2.729	2.729	2.730	2.730
50	2.731	2.732	2.733	2.734	2.735	2.737	2.738	2.740	2.741	2.743
51	2.745	2.747	2.749	2.751	2.753	2.755	2.758	2.760	2.763	2.766
52	2.769	2.772	2.775	2.778	2.782	2.785	2.788	2.792	2.795	2.799
53	2.803	2.807	2.811	2.815	2.820	2.824	2.828	2.833	2.838	2.843
54	2.848	2.853	2.858	2.863	2.868	2.874	2.879	2.885	2.890	2.896
55	2.902	2.908	2.914	2.921	2.927	2.933	2.940	2.946	2.953	2.960
56	2.967	2.974	2.981	2.988	2.996	3.004	3.011	3.019	3.026	3.034
57	3.042	3.050	3.059	3.067	3.075	3.084	3.092	3.101	3.110	3.119
58	3.128	3.137	3.147	3.156	3.166	3.175	3.185	3.195	3.205	3.215
59	3.225	3.235	3.246	3.256	3.267	3.278	3.289	3.300	3.311	3.322
60	3.333	3.345	3.356	3.368	3.380	3.392	3.404	3.416	3.429	3.441
61	3.454	3.466	3.479	3.492	3.505	3.518	3.532	3.545	3.559	3.573
62	3.587	3.601	3.615	3.629	3.643	3.658	3.673	3.688	3.703	3.718
63	3.733	3.749	3.764	3.780	3.796	3.812	3.828	3.844	3.861	3.878
64	3.894	3.911	3.928	3.946	3.963	3.980	3.998	4.016	4.034	4.052
65	4.071	4.090	4.108	4.127	4.147	4.166	4.185	4.205	4.225	4.245
66	4.265	4.285	4.306	4.327	4.348	4.369	4.390	4.412	4.434	4.456
67	4.478	4.500	4.523	4.546	4.569	4.592	4.616	4.640	4.664	4.688
68	4.712	4.737	4.762	4.787	4.812	4.838	4.864	4.890	4.916	4.943
69	4.970	4.997	5.024	5.052	5.080	5.109	5.137	5.166	5.195	5.224
70	5.254	5.284	5.315	5.345	5.376	5.408	5.440	5.471	5.504	5.536
71	5.569	5.602	5.636	5.670	5.705	5.740	5.775	5.810	5.846	5.883
72	5.919	5.956	5.994	6.032	6.071	6.109	6.149	6.189	6.229	6.270
73	6.311	6.352	6.394	6.437	6.480	6.524	6.568	6.613	6.658	6.703
74	6.750	6.797	6.844	6.892	6.941	6.991	7.041	7.091	7.142	7.194
75	7.247	7.300	7.354	7.409	7.465	7.521	7.578	7.636	7.694	7.753
76	7.813	7.874	7.936	7.999	8.063	8.128	8.193	8.259	8.327	8.395
77	8.465	8.536	8.607	8.680	8.754	8.829	8.905	8.982	9.061	9.142
78	9.223	9.305	9.389	9.474	9.561	9.649	9.739	9.831	9.924	10.02
79	10.12	10.21	10.31	10.41	10.52	10.62	10.73	10.84	10.95	11.06
80	11.18	11.30	11.42	11.54	11.67	11.80	11.93	12.06	12.20	12.34
81	12.48	12.63	12.78	12.93	13.08	13.24	13.40	13.57	13.74	13.92
82	14.10	14.28	14.47	14.66	14.86	15.07	15.28	15.49	15.71	15.94
83	16.17	16.41	16.66	16.91	17.17	17.44	17.72	18.01	18.31	18.61
84	18.93	19.25	19.59	19.94	20.30	20.68	21.07	21.47	21.89	22.32
85	22.77	23.24	23.73	24.24	24.78	25.34	25.92	26.52	27.16	27.83
86	28.53	29.27	30.04	30.86	31.73	32.64	33.60	34.63	35.72	36.88
87	38.11	39.43	40.84	42.36	44.00	45.76	47.68	49.76	52.02	54.50

From Henry, Lipson, and Wooster [G.8].

4

APPENDIX 15

DATA FOR CALCULATION OF THE TEMPERATURE FACTOR

Values of $\phi(x) = \frac{1}{x}\int_0^x \frac{\xi}{e^\xi - 1}\,d\xi$ as a Function of x

x	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9
0	1.000	0.975	0.951	0.928	0.904	0.882	0.860	0.839	0.818	0.797
1	0.778	0.758	0.739	0.721	0.703	0.686	0.669	0.653	0.637	0.622
2	0.607	0.592	0.578	0.565	0.552	0.539	0.526	0.514	0.503	0.491
3	0.480	0.470	0.460	0.450	0.440	0.431	0.422	0.413	0.404	0.396
4	0.388	0.380	0.373	0.366	0.359	0.352	0.345	0.339	0.333	0.327
5	0.321	0.315	0.310	0.304	0.299	0.294	0.289	0.285	0.280	0.276
6	0.271	0.267	0.263	0.259	0.255	0.251	0.248	0.244	0.241	0.237

For x greater than 7, $\phi(x)$ is given to a good approximation by $(1.642/x)$. (From Vol. 2, p. 264 of [G.11]).

Debye Temperatures

James [G.7, p. 221] gives the following values of the characteristic Debye temperature Θ for some cubic metals.

Metal	Θ(°K)	Metal	Θ(°K)
Al	390	Ta	245
Ca	230	Pb	88
Cu	320	Fe	430
Ag	210	Co	410
Au	175	Ni	400
Cr	485	Pd	275
Mo	380	Ir	285
W	310	Pt	230

APPENDIX 16

ATOMIC WEIGHTS

Based on the assigned relative atomic mass of $^{12}C = 12$.

Element	Symbol	Atomic number	Atomic weight
Actinium	Ac	89	(227)
Aluminium	Al	13	26.9815
Americium	Am	95	(243)
Antimony	Sb	51	121.75
Argon	Ar	18	39.948
Arsenic	As	33	74.9216
Astatine	At	85	(210)
Barium	Ba	56	137.34
Berkelium	Bk	97	(247)
Beryllium	Be	4	9.01218
Bismuth	Bi	83	208.9806
Boron	B	5	10.81
Bromine	Br	35	79.904
Cadmium	Cd	48	112.40
Calcium	Ca	20	40.08
Californium	Cf	98	(249)
Carbon	C	6	12.011
Cerium	Ce	58	140.12
Cesium	Cs	55	132.9055
Chlorine	Cl	17	35.453
Chromium	Cr	24	51.996
Cobalt	Co	27	58.9332
Copper	Cu	29	63.546
Curium	Cm	96	(247)
Dysprosium	Dy	66	162.50
Einsteinium	Es	99	(254)
Erbium	Er	68	167.26
Europium	Eu	63	151.96
Fermium	Fm	100	(253)
Fluorine	F	9	18.9984
Francium	Fr	87	(223)
Gadolinium	Gd	64	157.25
Gallium	Ga	31	69.72
Germanium	Ge	32	72.59
Gold	Au	79	196.9665
Hafnium	Hf	72	178.49
Helium	He	2	4.00260
Holmium	Ho	67	164.9303
Hydrogen	H	1	1.0080
Indium	In	49	114.82
Iodine	I	53	126.9045
Iridium	Ir	77	192.22
Iron	Fe	26	55.847
Krypton	Kr	36	83.80
Lanthanum	La	57	138.9055
Lawrencium	Lr	103	(257)
Lead	Pb	82	207.2
Lithium	Li	3	6.941
Lutetium	Lu	71	174.97
Magnesium	Mg	12	24.305
Manganese	Mn	25	54.9380
Mendelevium	Md	101	(256)
Mercury	Hg	80	200.59
Molybdenum	Mo	42	95.94
Neodymium	Nd	60	144.24
Neon	Ne	10	20.179
Neptunium	Np	93	237.0482
Nickel	Ni	28	58.71
Niobium	Nb	41	92.9064
Nitrogen	N	7	14.0067
Nobelium	No	102	(254)
Osmium	Os	76	190.2
Oxygen	O	8	15.9994
Palladium	Pd	46	106.4
Phosphorus	P	15	30.9738
Platinum	Pt	78	195.09
Plutonium	Pu	94	(242)
Polonium	Po	84	(210)
Potassium	K	19	39.102
Praseodymium	Pr	59	140.9077
Promethium	Pm	61	(147)
Protactinium	Pa	91	231.0359
Radium	Ra	88	226.0254
Radon	Rn	86	(222)
Rhenium	Re	75	186.2
Rhodium	Rh	45	102.9055
Rubidium	Rb	37	85.4678
Ruthenium	Ru	44	101.07
Samarium	Sm	62	150.4
Scandium	Sc	21	44.9559
Selenium	Se	34	78.96
Silicon	Si	14	28.086
Silver	Ag	47	107.868
Sodium	Na	11	22.9898
Strontium	Sr	38	87.62
Sulfur	S	16	32.06
Tantalum	Ta	73	180.9479
Technetium	Tc	43	98.9062
Tellurium	Te	52	127.60
Terbium	Tb	65	158.9254
Thallium	Tl	81	204.37
Thorium	Th	90	232.0381
Thulium	Tm	69	168.9342
Tin	Sn	50	118.69
Titanium	Ti	22	47.90
Tungsten	W	74	183.85
Uranium	U	92	238.029
Vanadium	V	23	50.9414
Xenon	Xe	54	131.30
Ytterbium	Yb	70	173.04
Yttrium	Y	39	88.9059
Zinc	Zn	30	65.37
Zirconium	Zr	40	91.22

Values in parentheses represent the most stable known isotopes.