Final Examination
2018/2019 Academic Session

June 2019

JIK420 – Advanced Physical Chemistry
(Kimia Fizik Lanjutan)

Duration : 3 hours
(Masa : 3 jam)

Please check that this examination paper consists of **FIFTEEN (15)** pages of printed material before you begin the examination.

*[Sila pastikan bahawa kertas peperiksaan ini mengandungi **LIMA BELAS (15)** muka surat yang bercetak sebelum anda memulakan peperiksaan ini].*

Instructions : Answer **FIVE (5)** questions. Answer the questions in English. You may also answer the questions in Bahasa Malaysia, but not a mix of both languages.

*[**Arahan** : Jawab **LIMA (5)** soalan. Jawab soalan-soalan dalam Bahasa Inggeris. Anda juga dibenarkan menjawab soalan dalam Bahasa Malaysia, tetapi campuran antara kedua-dua bahasa ini tidak dibenarkan].*

In the event of any discrepancies, the English version shall be used.

[Sekiranya terdapat sebarang percanggahan pada soalan peperiksaan, versi Bahasa Inggeris hendaklah digunapakai].

1. (a). Differentiate between two mechanisms of X-ray production. Use figures to illustrate your answer.
Bezakan antara dua mekanisme pengeluaran sinar-X. Jelaskan jawapan anda dengan ilustrasi gambar rajah.

(6 marks/*markah*)

(b). Sketch an X-ray tube and explain how Thermionic emission related to X-ray generation.
Lakarkan tiub sinar-X dan terangkan bagaimana pelepasan Thermionik yang berkaitan dengan penjanaan sinar-X.

(6 marks/*markah*)

(c). Compare and contrast constructive and destructive interference of reflected X-ray beams through crystals. Use figures to illustrate your answer.
Banding dan bezakan interferens membina dan interferens memusnah sinar-X yang dipantulkan melalui hablur. Jelaskan jawapan anda dengan ilustrasi gambar rajah.

(8 marks/*markah*)

2. (a). To determine an unknown crystal structure, which of the following techniques can be used?
Untuk menentukan struktur hablur yang tidak diketahui, teknik yang manakah boleh berikut digunakan?

(i). The Laue technique.
Teknik Laue.

(ii). A single crystal diffractometer.
Pembelauan hablur tunggal.

Justify your answer with reasons?
Jelaskan jawapan anda dengan alasan?

(4 marks/*markah*)

(b). A crystal has a lattice spacing of 0.314 nm and exhibits its first order X-ray diffraction at 12.8 degrees. What is the energy of the photons that were diffracted?

Suatu hablur mempunyai jarak kekisi 0.314 nm dan mempamerkan pembelauan sinar-X tertib pertama pada 12.8 darjah. Apakah tenaga foton yang dibelau?

(5 marks/*markah*)

(c). The copper metallic crystal with an atomic radius of 0.1278 nm has an FCC unit cell structure. The wavelength under the X-ray diffraction is 0.1542 nm. Calculate the diffraction angle θ for the crystallographic plane (111). Assume that the order of diffraction is 1st order.

Suatu hablur logam tembaga dengan jejari atom 0.1278 nm mempunyai struktur sel unit FCC. Panjang gelombang di bawah pembelauan sinar-X adalah 0.1542 nm. Hitung sudut pembelauan θ untuk satah kristalografi (111). Dengan anggapan bahawa tertib pembelauan adalah tertib pertama.

(7 marks/*markah*)

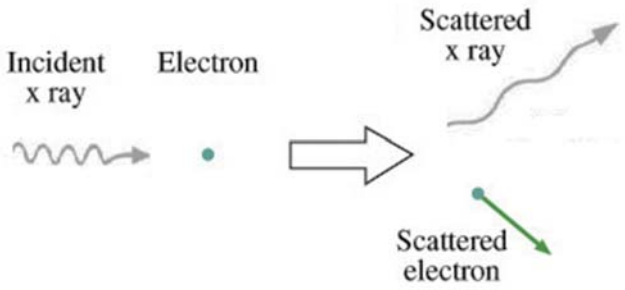


Figure 1
Rajah 1

(d). Consider the following diagram. Identify the mode of X-ray interaction that this figure depicts. How is this different from the other types of interactions?

Pertimbangkan gambar rajah berikut. Kenal pasti mod interaksi sinar-X yang digambarkan oleh gambar rajah ini. Bagaimana ia berbeza daripada jenis interaksi lain?

(4 marks/*markah*)

3. (a). Distinguish between stress and strain.
Bezakan tegasan dan terikan.

(5 marks/*markah*)

(b). Distinguish between elastic and plastic deformation.
Bezakan cacat bentuk kenyal dan plastic.

(5 marks/*markah*)

(c). How does chain branching affect the following properties of polyethylene:
Bagaimana pencabangan rantai boleh menjejaskan sifat polietilena berikut:

(i). amount of crystallinity,
jumlah kehabluran,

(ii). strength, and
kekuatan, dan

(iii). elongation?
pemanjangan?

(3 marks/*markah*)

(d). Define the glass transition temperature T_g?
Takrifkan suhu peralihan kaca Tg?

(2 marks/*markah*)

(e).

Polymer	Polyoxymethylene	Polyethylene	Polyvinyl chloride	Polystyrene
Structure	$-(OCH_2)_n-$	$-(C_2H_4)_n-$	$-(CH_2CHCl)_n-$	$-(CH_2-CH(C_6H_5)_n-$
T_g/K	198	253	354	381

The following table lists the glass transition temperatures, T_g, of several polymers. Discuss the reasons why the structure of the monomer unit has an effect on the value of T_g.
Jadual berikut menyenaraikan suhu peralihan kaca, Tg, beberapa polimer. Bincangkan sebab, struktur unit monomer mempunyai kesan ke atas nilai Tg.

(5 marks/*markah*)

...5/-

4. (a). Illustrate the following types of copolymers by using (○ & ●)for their mers:
Ilustrasikan jenis kopolimer berikut dengan menggunakan simbol (○ & ●):

(i). random,
rawak,

(ii). alternating,
selang-seli,

(iii). block, and
blok, dan

(iv). graft.
cangkuk.

(4 marks/*markah*)

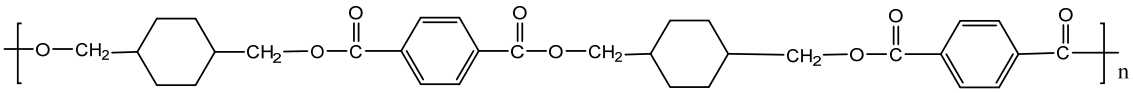
(b). Define stepwise polymerization of linear polymers. What by-products are commonly produced by stepwise polymerization?
Takrifkan langlah pempolimeran polimer linear. Apakah produk sampingan yang lazimnya dihasilkan oleh langkah pempolimeran begini?

(4 marks/*markah*)

(c). Write a chemical reaction for one molecule of a dibasic acid with a diamine to form an amide linkage. What is the by-product of this reaction?
Tuliskan reaksi kimia untuk satu molekul asid dwibes dengan diamina untuk membentuk rangkaian amida. Apakah hasil sampingan reaksi ini?

(6 marks/*markah*)

(d). Kodel is a polymer with the following structure:
[Kodel adalah polimer dengan struktur berikut]:



(i). Identify **TWO (2)** monomers for this structure.
*Kenal pasti **DUA (2)** monomer untuk struktur ini.*

(ii). Explain why this type of polymer is known as a condensation polymer
Jelaskan mengapa polimer jenis ini dikenali sebagai polimer kondensasi

(6 markah/*markah*)

5. (a). Describe the results of a photoelectric effect experiment. Which of those results cannot be explained by classical wave theory? How Einstein managed to explain the photoelectric effect?
Perihalkan keputusan-keputusan ujikaji kesan fotoelektrik. Keputusan manakah yang tidak boleh dijelaskan oleh teori gelombang klasik? Bagaimanakah Einstein berjaya menjelaskan kesan fotoelektrik?

(7 marks/*markah*)

(b). Show that the function $\sin 3x$ is an eigenfunction of the operator $\frac{d^2}{dx^2}$.

Tunjukkan bahawa fungsi sin $3x$ adalah suatu fungsi eigen bagi operator $\frac{d^2}{dx^2}$.

(5 marks/*markah*)

(c). According to quantum theory, the operator for energy is
Menurut teori kuantum, operator bagi tenaga ialah:

$$\hat{E} = -\frac{\hbar}{i}\frac{\partial}{\partial t}$$

where t *is the time.*
di sini t *ialah masa.*

(i). Derive the time-dependent wave function due to the following eigenvalue equation
Terbitkan fungsi gelombang bersandar masa yang disebabkan oleh persamaan nilai eigen berikut

$$-\frac{\hbar}{i}\frac{d}{dt}\psi(t) = E\psi(t)$$

where E *is the energy of the particle.*
di sini E *ialah tenaga zarah*.

(ii). Determine the probability density $|\psi|^2$ for the energy eigenfunction above. State the importance of this result for Chemistry.
Tentukan ketumpatan kebarangkalian $|\psi|^2$ *bagi fungsi eigen di atas. Nyatakan kepentingan keputusan ini bagi ilmu Kimia.*

(8 marks/*markah*)

6. (a). The wave function of a particle in a 1-dimensional box, where the potential is zero inside the box and infinite outside the box, is
Fungsi gelombang suatu zarah dalam suatu kotak 1-dimensi, yang mana keupayaannya sifar di dalam kotak dan infinit di luar kotak, ialah

$$\psi = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \qquad n = 1, 2, 3, \cdots$$

where n is the quantum number and a is the width of the box.
di sini n ialah nombor kuantum dan a ialah lebar kotak.

(i). Show that the average value of the momentum of the particle is zero. Explain.
Tunjukkan bahawa nilai purata momentum zarah itu adalah sifar. Jelaskan.

(ii). Derive an expression for the energy of the system.
Terbitkan suatu ungkapan bagi tenaga sistem tersebut.

(10 marks/*markah*)

(b). The Hamiltonian for a particle of mass m in a 2-dimensional box is given by
Hamiltonian bagi suatu zarah berjisim m dalam suatu kotak 2-dimensi diberikan oleh

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)$$

and the allowed wave function for the system is
dan fungsi gelombang yang dibenarkan bagi sistem itu ialah

$$\psi_{n_x n_y} = \left(\frac{4}{ab}\right)^{1/2} \sin\frac{n_x \pi x}{a} \sin\frac{n_y \pi y}{b}$$

where n_x and n_y are the quantum numbers and a and b are the box dimensions. Derive the allowed energies of this system.
di sini n_x dan n_y ialah nombor-nombor kuantum dan a dan b ialah dimensi kotak. Terbitkan tenaga-tenaga yang dibenarkan bagi sistem ini.

(10 marks/*markah*)

Constants:

Speed of light $c = 3.0 \times 10^{8}$ m s^{-1}

Avogadro's number $N_A = 6.02 \times 10^{23}$ mol^{-1}

Planck constant $h = 6.63 \times 10^{-34}$ J s

Boltzmann constant $k = 1.38 \times 10^{-23}$ J K^{-1}

Permittivity of free space $\varepsilon_o = 8.85 \times 10^{-12}$ F m^{-1}

Permeability of free space $\mu_o = 4\pi \times 10^{-7}$ H m^{-1}

Basic charge $e = 1.6 \times 10^{-19}$ C

Electron rest-mass $m_e = 9.1 \times 10^{-31}$ kg

Proton rest-mass $m_p = 1.6725 \times 10^{-27}$ kg $\equiv$ 1.0072766 u

Neutron rest-mass $m_n = 1.6748 \times 10^{-27}$ kg $\equiv$ 1.0086654 u

Bohr's radius $a = 5.3 \times 10^{-11}$ m

1 eV = 1.6×10^{-19} J

1 u $\equiv$ 931 MeV c^{-2}

1 barn = 10^{-28} m^2

1 fm = 10^{-15} m

1 Ci = 3.7×10^{10} s^{-1}

USEFUL MATHEMATICS IN QUANTUM MECHANICS

Exponential series

$$e^{x} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \cdots + \frac{x^n}{n!}$$

$$e^{ix} = \cos x + i \sin x$$

$$e^{-ix} = \cos x - i \sin x$$

Trigonometric series

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots$$

$$\tan x = x + \frac{x^3}{3} + \frac{2x^5}{15} + \cdots$$

Binomial expansion

$$(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 + \cdots$$

Differentiation and integration (Standard forms)

Differentiation	Integration
$\frac{d}{dx}x^n = nx^{n-1}$ $\frac{d}{dx}(ax+b)^n = na(ax+b)^{n-1}$	$\int x^n dx = \frac{x^{n+1}}{n+1} + c$ $\int (ax+b)^n dx = \frac{(ax+b)^{n+1}}{a(n+1)} + c$
$\frac{d}{dx}\log x = \frac{1}{x}$ $\frac{d}{dx}\log(ax+b) = \frac{a}{ax+b}$	$\int \frac{dx}{x} = \log x + c$ $\int \frac{dx}{ax+b} = \frac{1}{a}\log(ax+b) + c$
$\frac{d}{dx}e^x = e^x$ $\frac{d}{dx}e^{mx} = me^{mx}$	$\int e^x dx = e^x + c$ $\int e^{mx} dx = \frac{e^{mx}}{m} + c$
$\frac{d}{dx}\sin x = \cos x$ $\frac{d}{dx}\sin mx = m\cos mx$	$\int \cos x\, dx = \sin x + c$ $\int \cos mx\, dx = \frac{\sin mx}{m} + c$
$\frac{d}{dx}\cos x = -\sin x$ $\frac{d}{dx}\cos mx = -m\sin mx$	$\int \sin x\, dx = -\cos x + c$ $\int \sin mx\, dx = -\frac{\cos mx}{m} + c$
$\frac{d}{dx}\tan x = \sec^2 x$ $\frac{d}{dx}\tan mx = m\sec^2 mx$	$\int \sec^2 x\, dx = \tan x + c$ $\int \sec^2 mx\, dx = \frac{\tan mx}{m} + c$
$\frac{d}{dx}\cot x = -\text{cosec}^2 x$ $\frac{d}{dx}\cot mx = -m\ \text{cosec}^2 mx$	$\int \text{cosec}^2 x\, dx = -\cot x + c$ $\int \text{cosec}^2 mx\, dx = -\frac{\cot mx}{m} + c$
$\frac{d}{dx}\sinh x = \cosh x$	$\int \cosh x\, dx = \sinh x + c$
$\frac{d}{dx}\cosh x = \sinh x$	$\int \sinh x\, dx = \cosh x + c$

...13/-

Integration by parts

$$\int u\upsilon\, dx = u\int \upsilon\, dx - \int \left\{\int \upsilon\, dx\right\}\frac{du}{dx}dx$$

Integration common in Quantum Mechanics

$$f(x) = \int_0^\infty x^n e^{-ax^2} dx$$

n	$f(x)$	n	$f(x)$
0	$\frac{1}{2}\sqrt{\frac{\pi}{a}}$	1	$\frac{1}{2a}$
2	$\frac{1}{4}\sqrt{\frac{\pi}{a^3}}$	3	$\frac{1}{2a^2}$
4	$\frac{3}{8}\sqrt{\frac{\pi}{a^5}}$	5	$\frac{1}{a^3}$
6	$\frac{15}{16}\sqrt{\frac{\pi}{a^7}}$	7	$\frac{3}{a^4}$

If *n* is even, $\int_{-\infty}^{\infty} x^n e^{-ax^2} dx = 2f(x)$

If *n* is odd, $\int_{-\infty}^{\infty} x^n e^{-ax^2} dx = 0$

Other standard integrals

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

$$\int_0^\infty \frac{x}{\left(e^x - 1\right)} dx = \frac{\pi^2}{6}$$

$$\int_0^\infty \frac{x^3}{\left(e^x - 1\right)} dx = \frac{\pi^4}{15}$$

Pythagorean identities

$$\sin^2 u + \cos^2 u = 1$$
$$1 + \tan^2 u = \sec^2 u$$
$$1 + \cot^2 u = \csc^2 u$$

Sum & difference formulas

$$\sin(u \pm \upsilon) = \sin u \cos \upsilon \pm \cos u \sin \upsilon$$
$$\cos(u \pm \upsilon) = \cos u \cos \upsilon \mp \sin u \sin \upsilon$$
$$\tan(u \pm \upsilon) = \frac{\tan u \pm \tan \upsilon}{1 \mp \tan u \tan \upsilon}$$

Double angle formulas

$$\sin(2u) = 2 \sin u \cos u$$
$$\cos(2u) = \cos^2 u - \sin^2 u$$
$$= 2\cos^2 u - 1$$
$$= 1 - 2\sin^2 u$$
$$\tan(2u) = \frac{2 \tan u}{1 - \tan^2 u}$$

Power reducing/half angle formulas

$$\sin^2 u = \frac{1 - \cos(2u)}{2}$$
$$\cos^2 u = \frac{1 + \cos(2u)}{2}$$
$$\tan^2 u = \frac{1 - \cos(2u)}{1 + \cos(2u)}$$

Sum-to-product formulas

$$\sin u + \sin \upsilon = 2\sin\left(\frac{u+\upsilon}{2}\right)\cos\left(\frac{u-\upsilon}{2}\right)$$

$$\sin u - \sin \upsilon = 2\cos\left(\frac{u+\upsilon}{2}\right)\sin\left(\frac{u-\upsilon}{2}\right)$$

$$\cos u + \cos \upsilon = 2\cos\left(\frac{u+\upsilon}{2}\right)\cos\left(\frac{u-\upsilon}{2}\right)$$

$$\cos u - \cos \upsilon = -2\sin\left(\frac{u+\upsilon}{2}\right)\sin\left(\frac{u-\upsilon}{2}\right)$$

Product-to-sum formulas

$$\sin u \sin \upsilon = \frac{1}{2}\left[\cos(u-\upsilon) - \cos(u+\upsilon)\right]$$

$$\cos u \cos \upsilon = \frac{1}{2}\left[\cos(u-\upsilon) + \cos(u+\upsilon)\right]$$

$$\sin u \cos \upsilon = \frac{1}{2}\left[\sin(u+\upsilon) + \sin(u-\upsilon)\right]$$

$$\cos u \sin \upsilon = \frac{1}{2}\left[\sin(u+\upsilon) - \sin(u-\upsilon)\right]$$

- oooOooo -