L-Università ta' Malta

Department of Chemistry
Faculty of Science

B.Sc. (Hons.) Year I

Sample Examination Paper II

CHE1215: Methods of Chemical Calculations

*n*th June 20XX
08:30–11:35

Instructions

Read the following instructions carefully.

- Attempt only **TEN** questions.
- Each question carries **10** marks. The maximum mark is **100**.
- A list of mathematical formulae is provided on page 2.
- Only the use of non-programmable calculators is allowed.

MATHEMATICAL FORMULÆ

ALGEBRA

Factors

$$a^3 + b^3 = (a+b)(a^2 - ab + b^2)$$
$$a^3 - b^3 = (a-b)(a^2 + ab + b^2)$$

Quadratics

If $ax^2 + bx + c$ has roots α and β,

$$\Delta = b^2 - 4ac$$
$$\alpha + \beta = -\tfrac{b}{a} \qquad \alpha\beta = \tfrac{c}{a}$$

Finite Series

$$\sum_{k=1}^{n} 1 = n \qquad \sum_{k=1}^{n} k = \frac{n(n+1)}{2}$$
$$\sum_{k=1}^{n} k^2 = \frac{k(k+1)(2k+1)}{6}$$
$$(1+x)^n = \sum_{k=0}^{n} \binom{n}{k} x^n$$
$$= 1 + nx + \tfrac{n(n-1)}{2\cdot 1} x^2 + \cdots + x^n$$

GEOMETRY & TRIGONOMETRY

Distance Formula

If $A = (x_1, y_1)$ and $B = (x_2, y_2)$,

$$d(A,B) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$
$$= \sqrt{\Delta x^2 + \Delta y^2}$$

Pythagorean Identity

$$\cos^2\theta + \sin^2\theta = 1$$

General Solutions

$$\cos\theta = \cos\alpha \iff \theta = \pm\alpha + 2\pi\mathbb{Z}$$
$$\sin\theta = \sin\alpha \iff \theta = (-1)^n\alpha + \pi n,\ n \in \mathbb{Z}$$
$$\tan\theta = \tan\alpha \iff \theta = \alpha + \pi\mathbb{Z}$$

CALCULUS

Derivatives

$f(x)$	$f'(x)$
x^n	nx^{n-1}
$\sin x$	$\cos x$
$\cos x$	$-\sin x$
$\tan x$	$\sec^2 x$
$\cot x$	$-\operatorname{cosec}^2 x$
$\sec x$	$\sec x \tan x$
$\operatorname{cosec} x$	$-\operatorname{cosec} x \cot x$
e^x	e^x
$\log x$	$1/x$
uv	$u'v + uv'$
u/v	$(u'v - uv')/v^2$

Integrals

$f(x)$	$\int f(x)\,dx$
$x^n\ (n \neq -1)$	$\frac{x^{n+1}}{n+1}$
$\sin x$	$-\cos x$
$\cos x$	$\sin x$
$\tan x$	$\log(\sec x)$
$\cot x$	$\log(\sin x)$
$\sec x$	$\log(\sec x + \tan x)$
$\operatorname{cosec} x$	$\log(\tan \frac{x}{2})$
e^x	e^x
$1/x$	$\log x$
$\frac{1}{a^2+x^2}$	$\frac{1}{a}\tan^{-1}\left(\frac{x}{a}\right)$
$\frac{x}{\sqrt{a^2+x^2}}$	$\sin^{-1}\left(\frac{x}{a}\right)$

Homogeneous Linear Second Order ODEs

If the roots of $ak^2 + bk + c$ are k_1 and k_2, then the differential equation $ay'' + by' + cy = 0$ has general solution

$$y(x) = \begin{cases} c_1 e^{k_1 x} + c_2 e^{k_2 x} & \text{if } k_1 \neq k_2 \\ c_1 e^{kx} + c_2 x e^{kx} & \text{if } k = k_1 = k_2 \\ e^{\alpha x}(c_1 \cos\beta x + c_2 \sin\beta x) & \text{if } k = \alpha \pm \beta i \in \mathbb{C} \end{cases}$$

Infinite Series

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \frac{x^4}{4!} \cdots$$
$$\cos x = \sum_{\substack{n=0 \\ n \text{ even}}}^{\infty} \frac{(-1)^{\frac{n}{2}}}{n!} x^n = 1 - \frac{x^2}{2} + \frac{x^4}{4!} - \cdots$$
$$\sin x = \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} \frac{(-1)^{\frac{n-1}{2}}}{n!} x^n = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots$$
$$\log(1+x) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} x^n = x - \frac{x^2}{2} + \frac{x^2}{3} - \cdots, \quad x \in (-1, 1]$$

⚠ Attempt only **TEN** questions.

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1. (a) The Schrödinger equation for a particle inside a one-dimensional box is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = E\Psi,$$

where $\hbar$, m and E have their usual meaning and can be treated as constants for this question. Show that this has general solution

$$\Psi(x) = c_1\cos(\omega x) + c_2\sin(\omega x),$$

where $\omega^2 = 2mE/\hbar^2$.

(b) The rate law of the reaction $A \longrightarrow P$ following first order kinetics with respect to $[A]$ is given by

$$-\frac{d[A]}{dt} = k[A],$$

where $[A]$ is the concentration of A at time t after the start of the reaction, and k is the rate constant. Show that

$$[A] = [A]_0\exp(-kt)$$

if $[A] = [A]_0$ at time $t = 0$.

[5, 5 marks]

2. (a) Solve the equation $(x+2)^2(x+5) = 4$.

(b) Sketch the graphs $y = (x+2)^2$ and $y = \dfrac{4}{x+5}$ on the same axes.

(c) Find the area bounded by the two curves in (b) between their points of intersection.

[4, 3, 3 marks]

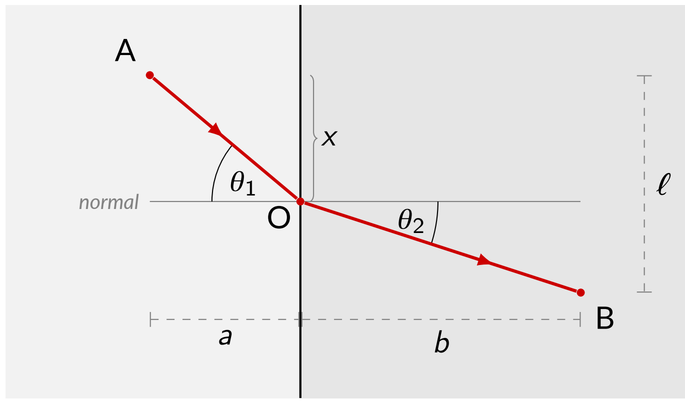
3. Solve the differential equation

$$2\sqrt{x}\frac{dy}{dx} = (y^2+1)(x+1)(5x-2), \qquad \text{where} \qquad y'(0) = 0.$$

Express your solution in the form $y(x) = \tan(\sqrt{x}(ax^2+bx+c))$.

[10 marks]

4. Consider a ray of light passing from one medium to another.



Given that light passes through medium 1 with velocity v_1, and through medium 2 with velocity v_2, show that the total time taken to travel from A to B through the variable point O is

$$T(x) = \frac{\sqrt{a^2 + x^2}}{v_1} + \frac{\sqrt{b^2 + (\ell - x)^2}}{v_2}.$$

Fermat's principle states that light travels the path which takes the least time. Assuming this principle, deduce *Snell's law*:

$$\frac{\sin\theta_1}{v_1} = \frac{\sin\theta_2}{v_2}.$$

[10 marks]

5. Consider the function

$$F(x,y,z) = x^2 \sin y + y \tan z + xy + 1.$$

(a) Find the partial derivatives $\frac{\partial F}{\partial x}$, $\frac{\partial F}{\partial y}$ and $\frac{\partial F}{\partial z}$.

(b) Find the Laplacian $\nabla^2 F = \frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} + \frac{\partial^2 F}{\partial z^2}$.

(c) Find the total differential dF, hence show that near $(1,0,\pi)$,

$$F(x,y,z) \approx \pi x + y + z - \pi + 1.$$

[3, 3, 4 marks]

6. Consider the curve given by the equation

$$y = \frac{(x-1)^3}{\sqrt{e^x}}$$

(a) Determine the coordinates of stationary points on the curve.

(b) Determine their nature.

(c) Sketch the curve, labelling any turning points and intercepts with the x- and y-axes.

[3, 4, 3 marks]

7. (a) Find the derivatives of the following functions.

(i) $\log\left(\frac{\sqrt[3]{2x}\,\sqrt[4]{4x^3}}{\sqrt{x^2-1}}\right)$ (ii) $e^x \tan(x^2)$ (iii) $\frac{\cos(x^2)}{\sqrt{1+\sin(x^2)}}$

(b) Verify that $y(x) = e^{2x^2}$ is a solution to the second order differential equation $xy'' = y' + 16x^3 y$.

[6, 4 marks]

8. Find the following integrals.

(a) $\int \frac{4x-5}{(x^2-x+1)(2x+1)}\,dx$ (b) $\int_0^{\pi} \cos\left(\frac{\theta-\pi}{6}\right) d\theta$ (c) $\int_2^{2\sqrt{3}} \frac{x+1}{x(x^2+4)}\,dx$

[3, 3, 4 marks]

9. Consider the trigonometric function $f(\theta) = 2\sin(2\theta + \frac{\pi}{3})$.

(a) Sketch $y = f(\theta)$ for $0 \leqslant \theta \leqslant 2\pi$.

(b) Solve the equation $f(\theta) + 1 = 0$ for $0 \leqslant \theta \leqslant 2\pi$.

(c) Indicate your solutions on your sketch from part (a), and also illustrate them on a sketch of the unit circle.

[4, 4, 2 marks]

10. Solve the differential equation

$$y'' - 4y' - 5y = 36e^{5x},$$

given that when $x = 0$, y and y' are both 0. **[10 marks]**

11. (a) The matrix **R** represents a rotation through an angle of $180°$, and the matrix **T** represents a reflection in the line $y = -x$.

(i) Write down the matrices **R** and **T**.

(ii) What does the matrix **RT** represent?

(b) Consider the matrices

$$\mathbf{A} = \begin{pmatrix} 0 & 4 & 1 \\ 1 & 5 & 2 \\ 1 & 2 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} 1 & -2 & 3 \\ 1 & -1 & 1 \\ -3 & 4 & -4 \end{pmatrix}$$

Work out **AB**, hence solve the system of equations

$$\begin{cases} x - 2y + 3z = -3 \\ x - y + z = 0 \\ -3x + 4y - 4z = 1. \end{cases}$$

[4, 6 marks]

12. (a) Express the complex number $\zeta = 3 - \sqrt{3}i$ in the form $Re^{i\theta}$. Hence or otherwise, show that $(\zeta/2)^{12}$ is an integer.

(b) Consider the complex numbers $z = 3+2i$ and $w = 7-4i$. Determine:

(i) $11z - w$ (ii) zw (iii) w/z

(iv) $w^* + z^*$ (v) $|w^2|$ (vi) $\arg(11z - w)$

[4, 6 marks]

13. (a) The barometric formula $p = p_0 e^{-Mgh/RT}$ gives the pressure of a gas of molar mass M at altitude h, where p_0 is the pressure at sea level. Express T in terms of the other variables.

(b) Express $[H^+]$ in terms of the pH, where $\mathrm{pH} = -\log_{10}([H^+])$.

(c) Given that $\log a = 2$ and $e^b = 3$, evaluate:

(i) $a + b$ (ii) $\log \frac{a}{9} + 2b$ (iii) a^b (iv) $e^{b+\log(\log(a))}$

[3, 3, 4 marks]

14. (a) Sketch the following graphs.

(i) $y = 3\log\left(\frac{1}{x+1}\right)$ (ii) $y = \frac{x+1}{2x+1}$

(iii) $y = 5 - |5 - x|$

(b) Solve the equation $14^{3x-4} \cdot 15^{4-x} = 6^x \cdot 35^{4-x}$.

[6, 4 marks]

15. Let $f(x) = x^3 - 7x + 6$.

(a) On the same set of axes, sketch the graphs of:

(i) $y = f(x)$,

(ii) $y = f'(x)$,

(iii) $y = f''(x)$,

(iv) $y = f'''(x)$.

labelling any intercepts and turning points.

(b) Show that

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2}x^2 + \frac{f'''(0)}{6}x^3.$$

[7, 3 marks]