L-Università ta' Malta

Department of Chemistry
Faculty of Science

B.Sc. (Hons.) Year I

Sample Examination Paper III

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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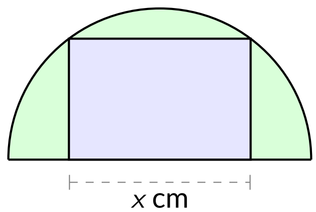
1. A rectangle is drawn inside a semicircle of radius 10 cm such that one if its sides, of length x cm, is along the diameter.



(a) Show that the area of the rectangle is

$$A(x) = \frac{x}{2}\sqrt{400 - x^2},$$

(b) Find the dimensions of the rectangle with the largest possible area.

(c) What is the green area in that case?

[4, 4, 2 marks]

2. (a) The rate law of the reaction A → P following first order kinetics with respect to $[A]$ is given by the equation $-\frac{d[A]}{dt} = k[A]$, where $[A]$ is the concentration of A at time t, and k is a constant. If $[A] = [A]_0$ when $t = 0$, show that

$$[A] = [A]_0 e^{-kt}.$$

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

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}[\Psi(x)] = E\Psi(x).$$

Show that this has solutions of the form

$$\Psi(x) = C\sin\left(\sqrt{\frac{2mE}{\hbar^2}}\,x\right),$$

given that $\Psi(0) = 0$.

[5, 5 marks]

3. (a) Show that $y = x\sin(2\log x)$ is a solution to $x^2\frac{d^2y}{dx^2} + 5y = x\frac{dy}{dx}$.

(b) Find the first, second and third derivatives of the function

$$f(x) = \log\left(\frac{\sqrt{2x}\,\sqrt[3]{3x}}{\sqrt[4]{4x+1}}\right).$$

[4, 6 marks]

4. Consider the matrices

$$\mathbf{A} = \begin{pmatrix} 1 & 2 \\ 1 & 1 \end{pmatrix} \qquad \text{and} \qquad \mathbf{B} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

(a) For each of them, state whether or not they have an inverse, and if so, find it.

(b) Work out $(\mathbf{A}+\mathbf{B})^2$ and $\mathbf{A}^2 + 2\mathbf{AB} + \mathbf{B}^2$. Are they equal? Why? [Recall the familiar rule $(a+b)^2 = a^2 + 2ab + b^2$ for numbers.]

(c) Solve the simultaneous equations

$$\begin{cases} x + 2y = 5 \\ x + y = 1 \end{cases}$$

using matrices.

(d) The matrix $\mathbf{C}$ represents an anticlockwise rotation by $30°$. Write down the matrix $\mathbf{C}^{51}$.

[3, 2, 2, 3 marks]

5. (a) Sketch the function $y = \tan(2x + \frac{\pi}{4})$ for $0 \leqslant x \leqslant \pi$.

(b) Solve the equation $3\tan^2(2x + \frac{\pi}{4}) = 1$ for $0 \leqslant x \leqslant \pi$.

(c) By superimposing a pair of appropriate lines on your sketch from part (a), illustrate your solutions to part (b) on the sketch.

[4, 4, 2 marks]

6. Solve the differential equation $y'' - 5y' + 6y = 2e^x$, given that when $x = 0$, y and y' are both 1.

[10 marks]

7. Consider the complex numbers

$$w = 2e^{i\pi/3} \qquad \text{and} \qquad z = \sqrt{3}w.$$

(a) Write down w and z in the form $a + bi$.

(b) Determine:

(i) wz	(ii) $2z^*/w$	(iii) $\arg(z+w)$
(iv) $\lvert z+w \rvert$	(v) $z + \frac{1}{w}$	(vi) z^8

(c) Write down 2^z in the form $a + bi$.

[2, 6, 2 marks]

8. Solve the differential equation

$$\cos^2 x \frac{dy}{dx} = y + 1,$$

given that $y = 4$ when $x = 0$. **[10 marks]**

9. Find the following integrals.

(a) $\displaystyle\int_1^4 \frac{1+x}{\sqrt{x}}$

(b) $\displaystyle\int \sec^2\left(3\theta + \tfrac{3\pi}{4}\right) d\theta$

(c) $\displaystyle\int_2^3 \frac{x+1}{(x-1)(x^2+1)}\, dx$

(d) $\displaystyle\int \frac{2x-3}{(x+1)(x^2+4)}\, dx$

[2, 1, 3, 4 marks]

10. Consider the curve given by

$$y = \frac{1+x}{1+x^2}.$$

(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-intercepts.

[3, 4, 3 marks]

11. (a) Solve the cubic equation $3x^3 + 2x^2 + 8x = 3$.

(b) Find the area bounded by $y = x^2 - 1$ and $y = 2 + x - x^2$.

[5, 5 marks]

12. (a) Given that $\log a = 2$, $\log b = 5$ and $\log c = 8$, evaluate:

(i) $\log a^2 b$ (ii) $\log_a b$

(iii) $\log b + \sqrt{\log \sqrt{c}}$ (iv) $\log \frac{a}{bc}$

(b) The Hyrdonium ion concentration $[H_3O^+]$ of an ammonia solution is around 0.00007. What is the pH value, to the nearest integer? [Recall that by definition of pH, $[H_3O^+] = 10^{-\mathrm{pH}}$.]

(c) If $\log(\log(\log x)) = 3$, what is x?

[4, 3, 3 marks]

13. The function f is given by

$$f(x,y) = x^2y^2 - xy - 2x + 3y + 1.$$

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

(b) Verify that the *Hessian*

$$H_f = \frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2$$

is $H_f = -(2xy-1)(6xy-1)$.

(c) Find the total differential df. Hence, show that for points close to $(1,2)$, we have the approximation

$$f(x,y) \approx 4x + 6y - 9.$$

[2, 4, 4 marks]

14. (a) Sketch the following graphs, labelling any x- and y-intercepts.

(i) $y = 1 - 2e^{2x}$ (ii) $y = 1 + 2\log(2x)$ (iii) $y = 3 + \sqrt{5-4x}$

(b) Solve the equation $\sqrt{\sqrt{\sqrt{x+1}+2}+3} = 4$.

[7, 3 marks]

15. The product of two positive numbers is the same as their average. What is the least possible value for the logarithm of the sum of their squares?

[10 marks]