UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For the following qualifications :-

B.Sc. *M.Sci.*

Mathematics B6: Mathematical Methods In Chemistry

COURSE CODE	:	**MATHB006**
UNIT VALUE	:	**0.50**
DATE	:	**20-MAY-02**
TIME	:	**14.30**
TIME ALLOWED	:	**2 hours**

02-C0897-3-40

© 2002 University of London

TURN OVER

All questions may be attempted but only marks obtained on the best **five** *solutions will count.*
The use of an electronic calculator is **not** *permitted in this examination.*

1. (a) Find the general solution of the differential equation

$$y'' - 4y' + 4y = \sinh x \cosh x.$$

(b) Using the substitution $x = e^t$, convert the differential equation

$$x^2y'' + xy' + y = 0,$$

into one with constant coefficients. Hence find the solution to the differential equation subject to the conditions $y = 2$ and $y' = 0$ when $x = 1$.

2. Verify that one solution of the differential equation

$$x^2\frac{d^2y}{dx^2} - x(x+2)\frac{dy}{dx} + (x+2)y = 0, \qquad (1)$$

is $y = x$.

By substituting $y = xu(x)$ into equation (1), show that $u(x)$ satisfies a second-order differential equation with constant coefficients. Hence find a second linearly independent solution to (1).

Substituting the series $y = \sum_{n=0}^{\infty} a_n x^n$ into (1), show that $a_0 = 0$ and a_1 is arbitrary. Derive a recurrence relation for the coefficients a_n for $n > 2$. Show that the series solution is the same as the solution found above.

3. (a) Legendre's differential equation is

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \alpha(\alpha+1)y = 0,$$

where α is a constant. By substituting the series $y = \sum_{n=0}^{\infty} a_n x^n$ into Legendre's equation derive the recurrence relation

$$a_{n+2} = \frac{(n-\alpha)(n+\alpha+1)}{(n+1)(n+2)} a_n,$$

for the coefficients a_n, $n \geq 0$. Deduce that there are two linearly independent solutions, one even and one odd, to Legendre's equation. If $\alpha = m$ is a positive integer, show that one of these series solutions is a polynomial of degree m, depending on whether m is even or odd.

(b) In spherical polar coordinates Laplace's equation for an axisymmetric function $u(r,\theta)$ is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial u}{\partial \theta}\right) = 0.$$

If solutions for ψ are sought in separable form $\psi = T(\theta)R(r)$, show that $T(\theta) = f(\cos\theta)$ where $y = f(x)$ satisfies Legendre's equation.

4. (a) Write down the generating function for Legendre polynomials $P_n(x)$. Use it to show that

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x).$$

Given that $P_0(x) = 1$ and $P_1(x) = x$, find $P_2(x)$ and $P_3(x)$.

(b) Given

$$\int_0^{\pi} \frac{dz}{A - iB\cos z} = \frac{\pi}{\sqrt{A^2+B^2}},$$

use the substitutions $A = 1 - \alpha\cos\theta$ and $B = \alpha\sin\theta$, where $0 < \alpha < 1$ and θ is real, and expand the integrand of the left-hand integral as a geometric series to show

$$P_n(\cos\theta) = \frac{1}{\pi}\int_0^{\pi} (\cos\theta + i\sin\theta\cos z)^n dz.$$

Use this integral formula to obtain $P_2(\cos\theta)$ in terms of $\cos\theta$.

5. (a) Write down the four axioms for a group G and state what is meant by saying G is Abelian.

   (b) In three-dimensional space denote by σ_{xz} the reflection in the xz plane, σ_{yz} the reflection in the yz-plane and r the rotation about the z-axis through π radians. Let I be the identity. Show that the four transformations $\{I, r, \sigma_{xz}, \sigma_{yz}\}$ form a group V_4, where the law of multiplying two elements together is to perform one transformation followed by the other.

   (c) Write down the multiplication table for a group W_4 of four elements which is not isomorphic to V_4. Which of the groups V_4 or W_4 is cyclic? Justify your answer.

6. (a) Define what is meant by a real symmetric matrix A. If $\mathbf{x}$ is a non-zero column vector (with possibly complex elements), show that $\bar{\mathbf{x}}^T A\mathbf{x}$ is real and that $\bar{\mathbf{x}}^T\mathbf{x}$ is real and positive, where $\bar{\mathbf{x}}$ denotes the complex conjugate of $\mathbf{x}$. Hence show that the eigenvalues of A are real.

   (b) Let $\mathbf{u}$ be a column vector with n elements and unit length. Show that the $n \times n$ matrix $\mathbf{u}\mathbf{u}^T$ is symmetric. Show also that the matrix $B = I - 2\mathbf{u}\mathbf{u}^T$ is orthogonal.

7. (a) Define what is meant by a unitary matrix U. If A is a unitary matrix and if $B = AP$, where P is non-singular, prove that PB^{-1} is unitary.

   (b) If A and B are unitary matrices of the same order, show that AB is unitary. Show that the set of all $n \times n$ unitary matrices form a group under matrix multiplication.

END OF PAPER